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UNIVERSITY OF BRISTOL

PHD THESIS

Semiclassical methods for investigating open quantum systems and decoherence

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Abstract

In this thesis we use the phase space formulation of quantum mechanics to investigate open quantum systems via the Lindblad equation [33][11] in the semiclassical limit with a focus on analysing the spread of decoherence. In the case of linear Lindblad operators and quadratic Hamiltonians where the phase space Lindblad equation becomes exact, we find that decoherence is intimately related to Hörmander's condition [20] which describes when a partial differential equation is hypoelliptic. In particular, it motivates a natural orthogonal decomposition of phase space which encodes the timescales describing the onset of decoherence as well as the subspaces which are protected. Explicit results for the evolution of a Gaussian coherent state and its Hilbert-Schmidt norm evolving under this exact Lindblad equation are given. We use this to investigate a class of simple examples of networks of harmonic oscillators and show that by changing the macro structure of the network, the spread of decoherence throughout the system can change dramatically. Finally, by interpreting the Lindblad equation as a Schrödinger equation on a doubled phase space, we use recent results in the theory of non-Hermitian Schrödinger equations [13][14] to determine the evolution of a Gaussian state under a Lindblad equation with general Hamiltonian and Lindblad operators.

Author's declaration

I declare that the work in this dissertation was carried out in accordance with the requirements of the University's Regulations and Code of Practice for Research Degree Programmes and that it has not been submitted for any other academic award. Except where indicated by specific reference in the text, the work is the candidate's own work. Work done in collaboration with, or with the assistance of, others, is indicated as such. Any views expressed in the dissertation are those of the author.

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Chapter 1

Introduction

Quantum mechanics has become well established through theory and rigorous experiment as one of the cornerstones of our current understanding of the natural world. At the turn of the 20th century, following the work of Einstein and Planck, it was found that the classical theories that had been used for centuries broke down at small scales. This was a revelation and led to a flurry of activity as the basis of what would become quantum theory was ironed out over the following decades. This was not a rejection of classical theory however, the predictions of classical mechanics were still incredibly accurate in the macroscopic regime, and thus, much as Newton's theory of gravity could be seen as a limit of Einstein's theory of gravitation, an interpretation of the classical world as a limit of quantum theory was sought.

This led, through the work of Wentzel, Kramers and Brillouin [8] when applied to the Schrödinger equation, to the concept of a semiclassical approximation, whereby expressions for quantum objects such as wave functions or energy levels are determined as functions of the reduced Planck's constant \hbar which are valid in the classical limit where $\hbar \rightarrow 0$. Parallel to this, due to the work of Weyl [48], Wigner [49], Groenewold [16] and Moyal [37] amongst others, the phase space formulation of quantum mechanics was developed which, through the invertible Wigner-Weyl map, allows one to relate functions on a classical phase space to operators on Hilbert space in the Schrödinger picture. The development of the rich theory of semiclassical analysis ensued which has been used extensively to investigate quantum mechanics as viewed from the phase space picture [51]. This phase space formulation of quantum mechanics will be the foundation of this thesis.

One of the main reasons quantum mechanics drew such interest was that it made predictions which were manifestly non-classical and, as the continuing philosophical debate about the interpretation of quantum mechanics shows, very unintuitive. A key feature of quantum mechanics is the existence of superpositions and entanglements of quantum states. These are concepts which are not classically observable and can be thought of as being purely 'quantum' in nature.

However these quantum entanglements, or equivalently quantum coherences, are known to decay rapidly upon interaction with an environment, in a process called quan-

tum decoherence [25]. Heuristically, decoherence can be thought of as the loss of information to the environment and in particular the loss of “quantum effects”. Decoherence occurs on incredibly rapid timescales and presents a continued challenge for the development of any quantum computer but also provides insight into the relationship between the quantum world and the classical world.

The focus of this thesis will be on using the tools of semiclassical theory and the study of open quantum systems to investigate the spread of decoherence and the timescales on which it occurs. We outline the structure of this thesis as follows.

In the first chapter we present a background on the theory we will need. We start by briefly describing the basic notation and quantum theory. We then introduce the well studied theory of density operators, in particular introducing the necessary concepts of trace class and Hilbert-Schmidt operators and culminating in the von-Neumann equation describing the time evolution of a density operator in a closed system, i.e. a system isolated from the environment.

Having reviewed the basic theory of closed quantum systems, we open up our system to environment effects. To this end we introduce the Lindblad equation [33][11]

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \frac{1}{2\hbar} \sum_j [\hat{L}_j \hat{\rho}, \hat{L}_j^\dagger] - [\hat{\rho} \hat{L}_j^\dagger, \hat{L}_j], \quad (1.0.1)$$

which can be thought of as the fundamental differential equation describing the evolution of a density operator in the presence of a Markovian environment. The full proof that the Lindblad equation is the fundamental equation describing such an evolution is based on semigroup theory which we will not use anywhere else in this thesis, hence we merely look to provide a constructive justification of its choice. Finally, we will discuss some examples of common choices of Lindblad operators (and hence Lindblad equations) governing various types of environment.

After introducing density operators and the Lindblad equation, we briefly review some other topics which we will need in what follows, in particular some basic symplectic geometry which will be underlying much of what we discuss in this thesis. From here we finally begin discussing the semiclassical theory that allows us to introduce the phase space description of quantum mechanics. In particular we introduce the Weyl quantization procedure [48] which allows us to associate an operator $\text{Op}(A)$ to a “symbol” $A(q, p)$ on phase space. From here we will introduce the \star product [16] which allows us to write the product of operators as

$$\hat{A}\hat{B} = \text{Op}(A)\text{Op}(B) = \text{Op}(A \star B) \quad (1.0.2)$$

where A and B are the phase space symbols associated to the operators \hat{A} and \hat{B} . We will then introduce the Wigner map and hence the Wigner function [49] (as well as the related characteristic function) which will finally allow us to represent the operator Lindblad equation (1.0.1) as the following symbol equation on phase space:

$$i\hbar \frac{\partial \rho}{\partial t} = H \star \rho - \rho \star H + i \sum_j L_j \star \rho \star \bar{L}_j - \frac{1}{2} \bar{L}_j \star L_j \star \rho - \frac{1}{2} \rho \star \bar{L}_j \star L_j. \quad (1.0.3)$$

In many ways this is the fundamental equation of study in this thesis. For general symbols H and L_k this equation can be given by a semiclassical expansion in powers of \hbar , but in the case where H is at most quadratic and the L_k at most linear in $x = (q, p)$ we have an exact evolution equation to second order in \hbar . This will be the assumption we make throughout the majority of this thesis.

Finally then for the background theory, we introduce Gaussian coherent states which are an overcomplete set of minimal uncertainty states which have the important property that the centres evolving under a Schrödinger equation closely follow the classical trajectories [5]. In particular we introduce the Wigner function of a Gaussian state as well as a superposition of Gaussian states which we will use extensively to investigate decoherence. We highlight this with a visual example of decoherence for a cat state, i.e. a superposition of two separated Gaussian coherent states, in a scattering environment.

Having covered the background theory, in Chapter 3 we will introduce some of the main results of this thesis. We restrict ourselves to the aforementioned exactly solvable case, where our Lindblad operators are at most linear and our Hamiltonian at most quadratic in x . The main result of this chapter can be described as showing that, in this exactly solvable situation, the spread of decoherence throughout our system due to the environment is fundamentally related to a condition from the theory of partial differential equations which guarantees the smoothness of solutions to PDEs, known as the Hörmander condition [20]. In particular, we will see that if this condition is satisfied then every part of the system experiences decoherence, but if it is not satisfied, there is some non-trivial subspace of our phase space which is protected.

We arrive at this result through a number of key insights. First and foremost, we use the fact that we can solve the exact Lindblad equation on phase space, or more exactly the Fourier transformed equation for the characteristic function $\chi(t, \xi)$. The form of this solution is

$$\chi(t, \xi) = \chi_0(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} \quad (1.0.4)$$

where the matrices R_t and D_t are related to the internal Hamiltonian dynamics of the system. R_t describes transport in the system and D_t provides a damping effect in the Fourier domain, which translates to a damping of oscillations in $\rho(t, x)$, which is a signifier of decoherence. Hence the quadratic form $D_t(\xi) = \xi \cdot D_t \xi$ can be thought of as determining decoherence in the system.

By applying this theory to cat states, and more generally the Wigner functions and characteristic functions associated to arbitrary superpositions of coherent states, we explore their evolution under the Lindblad equation and we can see the effect of decoherence directly. In particular, for a superposition of coherent states

$$\psi = \frac{1}{\sqrt{N}} \sum_{k=1}^N T_\Omega(y_k) \psi_0 \quad (1.0.5)$$

with Weyl symbol

$$\rho(t, x) = \frac{1}{N} \sum_{j,k=1}^N \rho_{jk}(t, x) \quad (1.0.6)$$

we determine explicit forms of the functions $\rho_{jk}(t, x)$ in terms of the initial symbol and the matrices R_t and D_t . Additionally, we provide an explicit expression for the Hilbert-Schmidt norm of the operators associated to these Weyl symbols. When applying these results to simple systems coupled to an environment we see clear evidence of the protected subspaces we alluded to earlier.

By rewriting the Lindblad equation in terms of a set of vector field X_0, X_k for $k = 1, \dots, 2K$ where K describes the total number of Lindblad operators, we consider Hörmander's condition, a condition guaranteeing hypoellipticity of a PDE, which ultimately reduces to checking whether there exists an $r \leq 2n - 1$ such that the vector space $V_r = \mathbb{R}^{2n}$ where

$$V_0 = \text{span}\{\text{Re } l_k, \text{Im } l_k \mid k = 1, \dots, K\} \quad (1.0.7)$$

and

$$V_j = V_0 + FV_0 + \dots + F^j V_0. \quad (1.0.8)$$

Here $F = \Omega H$ is the *Hamiltonian map* and the vectors l_k are (up to multiplication by the standard symplectic matrix Ω) the coefficients of the linear Lindblad symbols. Broadly then, this condition can be interpreted as checking whether the Hamiltonian dynamics of the system provide enough mixing to carry the influence of the environment, described by V_0 , to the entirety of phase space. If Hörmander's condition is not satisfied, there will exist some decoherence free subspace of the system. More than this, it also encodes information about the timescales upon which the effect of decoherence reaches the subspaces of the system.

There is a natural decomposition of phase space into a set of orthogonal subspaces W_k

$$\mathbb{R}^{2n} = W_0 \oplus W_1 \oplus \dots \oplus W_r \oplus W_{df} \quad (1.0.9)$$

where $W_0 = V_0$ and W_j is the orthogonal complement of V_{j-1} in V_j . Here we have included the *decoherence free* subspace W_{df} in this decomposition to allow for the situation in which Hörmander's condition is not satisfied. We see that the onset of decoherence in the system is described exactly by these subspaces, so that for instance an initial cat state centred in W_{j+1} will experience the onset of decoherence on a slower timescale than W_j and indeed if it is centred in W_{df} it will not experience it at all. We investigate this separation of timescales further by introducing some approximations of the matrices R_t and D_t , as well as some related quantities, which display the same short time behaviour and allow us to show this separation of timescales directly.

In the Chapter 4, we apply this theory to a set of simple examples, motivated initially by considering a chain of identical interacting harmonic oscillators, where one of the oscillators is coupled to an environment modelled as a heat bath. Such harmonic oscillator heat bath models are commonly studied in a variety of fields, from quantum field theory to molecular chemistry [23][43][26][19][39][10]. By considering the simple case of 3 oscillators, we see that if we couple the first oscillator to the environment we get full decoherence, and as we might expect, the effect of this decoherence travels down the chain of oscillators, so that states centred in the phase space corresponding to the

third oscillator decohere on a slower timescale than those on the second oscillator, and so on. However, if we choose instead to couple the middle oscillator to the environment, we find that there is a protected subspace of our overall phase space, given as a linear superposition of the first and third oscillators.

This observation inspires more investigation into models of this type, that is, systems which can be decomposed into networks of interacting subsystems with a graph-like structure. We present an algorithm which can be used to check the Hörmander condition for such systems and determine the orthogonal subspaces W_j and W_{df} . With some simplifying assumptions, this algorithm allows us to determine some general results for some basic structures, namely the chain, loop and star of N harmonic oscillators. These are some of the most fundamental networks but the algorithm holds more generally. It is hoped that these basic examples could serve as a basis for investigating the underlying symmetries of these graph like structures that results in the failure of Hörmander's condition and hence the introduction of decoherence free subspaces.

In the Chapter 5 we try to relax the assumption we made of linear Lindblad operators and quadratic Hamiltonians. In this case, our representation of the Lindblad equation on phase space is no longer exact and is instead an asymptotic expansion in \hbar hence we need a new tool set. We focus our efforts on understanding the evolution of Gaussian coherent states under the Lindblad equation in this more general situation.

The main idea of this chapter is to interpret the phase space Lindblad equation (1.0.3) as a Schrödinger equation on a doubled phase space, where our initial phase space point $x = (q, p)$ is interpreted as a 'position' and we have an associated 'momentum' y . In this way it can be written as

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}}(\hat{x}, \hat{y})\psi \quad (1.0.10)$$

where the Hamiltonian $\hat{\mathcal{H}}(\hat{x}, \hat{y})$ is determined from the observation that the star product can be written in operator form

$$A \star \psi = \hat{A}^{(-)}\psi, \quad \psi \star A = \hat{A}^{(+)}\psi \quad (1.0.11)$$

where the operators $\hat{A}^{(\pm)}$ are related to the symbol $A(x)$.

The resulting Hamiltonian is manifestly non-Hermitian, and as a result we apply some recent results from the theory of non-Hermitian Schrödinger equations in the case of Gaussian states [13][14]. This allows us to determine a set of equations describing the evolution of the centre, covariance matrix and overall phase of an initial coherent state under the influence of the phase space Lindblad equation with general H and L_k . This is an extension of previous results which were valid only for linear Lindblad operators [3].

Chapter 2

Background

2.1 Basic notation and introduction

We consider normalised quantum states on a Hilbert space \mathcal{H} represented in bracket notation by $|\psi\rangle \in \mathcal{H}$. As is usual, we have an inner product $\langle \cdot, \cdot \rangle$ defined on this Hilbert space which we will write in bracket notation as

$$\langle \phi, \psi \rangle = \langle \phi | \psi \rangle. \quad (2.1.1)$$

Operators acting on these states are denoted by letters with hats \hat{A}, \hat{x} etc. Where there is no ambiguity (as in what follows) we will drop the hats and represent them by simply upper case letters A, B . We will often use the outer product bracket notation

$$A |\psi\rangle = (|\phi\rangle \langle \psi|) |\psi\rangle = |\phi\rangle \quad (2.1.2)$$

or indeed the eigenstate decomposition of A

$$A = \sum_j a_j |a_j\rangle \langle a_j| \quad (2.1.3)$$

for self-adjoint A .

We can write a quantum state ψ in the position representation as

$$\psi(q) = \langle q | \psi \rangle. \quad (2.1.4)$$

Here $|q\rangle$ is a continuous position found as the eigenstate of the position operator \hat{q} with eigenvalue $q \in \mathbb{R}^n$:

$$\hat{q} |q\rangle = q |q\rangle. \quad (2.1.5)$$

Importantly, we have the following resolution of identity:

$$1 = \int_{\mathbb{R}^n} |q\rangle \langle q| dq. \quad (2.1.6)$$

The action of an operator A on a quantum state is described in the position representation by

$$(A\psi)(q) = \langle q|A|\psi\rangle. \quad (2.1.7)$$

In particular, it admits an integral kernel which we can see directly by using the resolution of identity for the position representation:

$$\int_{\mathbb{R}^n} \langle q|A|y\rangle \langle y|\psi\rangle dy = \int_{\mathbb{R}^n} K_A(q, y)\psi(y)dy, \quad (2.1.8)$$

where

$$K_A(q, y) := \langle q|A|y\rangle \quad (2.1.9)$$

is the integral kernel.

Similarly we can write an operator in the momentum representation

$$\tilde{\psi}(p) = \langle p|\psi\rangle \quad (2.1.10)$$

where the $|p\rangle$'s are eigenstates of the momentum operator \hat{p}

$$\hat{p}|p\rangle = p|p\rangle. \quad (2.1.11)$$

In the position representation the momentum operator \hat{p} operates on wave functions by differentiation:

$$\begin{aligned} \langle q|\hat{p}|\psi\rangle &= \langle q|\hat{p}\psi\rangle \\ &= (\hat{p}\psi)(q) \\ &= \left(\frac{\hbar}{i} \frac{\partial}{\partial q}\right) \psi(q). \end{aligned}$$

The inner product $\langle q|p\rangle$ is given by

$$\langle q|p\rangle = e^{\frac{i}{\hbar}q \cdot p} \quad (2.1.12)$$

and if we wish to change between position and momentum representations we see that

$$\begin{aligned} \tilde{\psi}(p) &= \langle p|\psi\rangle \\ &= \int_{\mathbb{R}^n} \langle p|q\rangle \langle q|\psi\rangle dq \\ &= \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}q \cdot p} \psi(q) dq \\ &= \mathcal{F}_h\{\psi\}(p) \end{aligned}$$

which is just the (semiclassical) Fourier transform of the position representation of $|\psi\rangle$ (more on this later).

The time evolution of a quantum state $|\psi\rangle$ is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt} |\psi\rangle = H |\psi\rangle \quad (2.1.13)$$

or in position representation

$$i\hbar \frac{\partial}{\partial t} \psi(q, t) = (H\psi)(q, t), \quad (2.1.14)$$

where the operator H is the Hamiltonian of the system. In the Schrödinger picture, time evolution of states $|\psi(t)\rangle = |\psi_t\rangle$ is described by the unitary operator U_t given by the operator exponential

$$U_t = \exp\left(-\frac{i}{\hbar} Ht\right) \quad (2.1.15)$$

acting on an initial state $|\psi(0)\rangle = |\psi_0\rangle$

$$|\psi_t\rangle = U_t |\psi_0\rangle. \quad (2.1.16)$$

2.2 Density operators

2.2.1 Trace class operators

In this section we will review the theory of trace class and Hilbert-Schmidt class operators. This section and how it relates to the following sections on semiclassics and quantization will be based heavily on the discussion in chapter 9 of [7] with slightly altered notation. Another useful review of these ideas is given in chapter 9 of [6]. Section 4, Chapter 8 in [44] also discusses trace class operators in detail without going into any semiclassical theory, and our discussion of density operators in the context of trace classes will be based upon this text.

We start by considering a general compact linear operator $A : E \rightarrow F$, denoted by $A \in \mathcal{B}(E, F)$ where E and F are two separable Hilbert spaces. In this situation $A^\dagger A$ and AA^\dagger are compact non-negative self-adjoint operators, where A^\dagger is the adjoint, with the same non-vanishing eigenvalues which we denote by $s_1(A)^2, s_2(A)^2, \dots$. In the case of infinitely many such values we have that $s_j(A) \rightarrow 0$ as $j \rightarrow \infty$ since A is compact. The $s_j(A)$ are the *characteristic* or *singular* values of A .

Definition 2.2.1. A is of *trace class* if

$$\|A\|_{tr} := \sum_{j=1}^{\infty} s_j(A) < \infty. \quad (2.2.1)$$

A is of *Hilbert-Schmidt class* if

$$\|A\|_{HS} := \left(\sum_{j=1}^{\infty} s_j(A)^2 \right)^{\frac{1}{2}} < \infty. \quad (2.2.2)$$

The spaces of Hilbert-Schmidt (HS) and trace class operators form Banach spaces (i.e. complete normed spaces). We also have that a bounded operator A is HS/trace

class if and only if A^* is HS/trace class. Note that the space of trace class operators is a subset of the space of Hilbert-Schmidt operators.

We also recall the operator norm of an operator acting on a normed vector space V

$$\|A\| = \inf\{c \geq 0 : \|Av\| \leq c\|v\|, \quad \forall v \in V\}. \quad (2.2.3)$$

We will now review some basic results for trace class operators.

Proposition 2.2.2 (Properties of trace class operators). *We have*

(i)

$$\|A\|_{tr} = \sup_{\{e_j\}, \{f_j\}} \sum_j |\langle Ae_j, f_j \rangle|, \quad (2.2.4)$$

for $\{e_j\}, \{f_j\}$ orthonormal bases of E and F respectively.

(ii) If B is a bounded operator and A is of trace class, then BA is trace class and

$$\|BA\|_{tr} \leq \|B\| \|A\|_{tr}. \quad (2.2.5)$$

Similarly, if C is bounded and A of trace class, then AC is trace class and

$$\|AC\|_{tr} \leq \|A\|_{tr} \|C\|. \quad (2.2.6)$$

(iii) If $A : E \rightarrow E$ is of trace class, then the trace defined as

$$\text{tr } A := \sum_j \langle e_j | A | e_j \rangle \quad (2.2.7)$$

is independent of the choice of ONB $\{e_j\}$ and we have

$$|\text{tr } A| \leq \|A\|_{tr} \quad (2.2.8)$$

(iv) If $A : E \rightarrow F$ is of trace class and $B : F \rightarrow E$ is bounded, then

$$\text{tr } AB = \text{tr } BA. \quad (2.2.9)$$

Finally we give some notation

Definition 2.2.3 (Notation). Given a Hilbert space \mathcal{H} we use the notation

$$A \in \mathcal{B}(\mathcal{H}) \quad (2.2.10)$$

to indicate that an operator A is in the set of all bounded linear operators acting on $\mathcal{H} \rightarrow \mathcal{H}$ and

$$A \in \mathcal{T}(\mathcal{H}) \quad (2.2.11)$$

for A in the set of all trace class operators acting on $\mathcal{H} \rightarrow \mathcal{H}$.

Lets give an important example.

Example 2.2.4. For an operator A given as in (2.1.2) by the outer product notation

$$A = |\phi\rangle \langle\psi| \quad (2.2.12)$$

we have that

$$\begin{aligned} \text{tr } A &= \text{tr } (|\phi\rangle \langle\psi|) \\ &= \sum_j \langle e_j | \phi \rangle \langle \psi | e_j \rangle \\ &= \langle \psi | \left(\sum_j |e_j\rangle \langle e_j| \right) | \phi \rangle \\ &= \langle \psi | \phi \rangle, \end{aligned}$$

where we have used the standard resolution of identity result.

For Hilbert-Schmidt operators we have the following properties:

Proposition 2.2.5 (Properties of HS operators). *We have*

- (i) *If $\{e_j\}$ and $\{f_j\}$ form orthonormal bases in E and F respectively, and $a_{jk} = \langle e_j | A | f_j \rangle$ are the corresponding matrix elements of A , then the HS norm is given by*

$$\|A\|_{HS}^2 = \sum_j \sum_k |a_{jk}|^2 = \sum_j \|Ae_j\|^2 = \sum_j \|A^\dagger f_j\|^2. \quad (2.2.13)$$

- (ii) *If $B \in \mathcal{B}(F, H)$ and A is HS, then BA is HS and*

$$\|BA\|_{HS} \leq \|B\| \|A\|_{HS}. \quad (2.2.14)$$

From the other side, if $C \in \mathcal{B}(D, E)$, and A is HS, then AC is HS and

$$\|AC\|_{HS} \leq \|A\|_{HS} \|C\|. \quad (2.2.15)$$

- (iii) *The HS operators $E \rightarrow F$ form a Hilbert space with scalar product $(A|B) = \text{tr } B^* A$.*

- (iv) *If we take $E = L^2(Y, \nu)$ and $F = L^2(Q, \mu)$ for $(Y, \nu), (Q, \mu)$ some measure spaces, then the operator $A : E \rightarrow F$ is HS if and only if A is an integral operator of the form*

$$Au(q) = \int K(q, y) u(y) \nu(dy) \quad (2.2.16)$$

where $K(q, y) \in L^2(Q \times Y; \mu \times \nu)$ is its Kernel. In such a case

$$\|K\|_{L^2} = \|A\|_{HS}. \quad (2.2.17)$$

We now remark upon the following direct result relating the kernel of an operator to the trace:

Proposition 2.2.6. *Suppose we have a trace class operator A acting on an $L^2(\mathbb{R}^n)$, then*

(i)

$$\mathrm{tr}(A) = \int K_A(q, q) dq, \quad (2.2.18)$$

(ii)

$$\mathrm{tr}(A^\dagger A) = \|K_A\|_{L^2}^2 = \|A\|_{HS}^2 \quad (2.2.19)$$

where K_A is the integral kernel of the operator A .

Proof. We start by using the definition of $\mathrm{tr} A$ (2.2.7) and inserting two resolutions of identity:

$$\begin{aligned} \mathrm{tr}(A) &= \sum_j \langle e_j | A | e_j \rangle \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_j \langle e_j | y \rangle \langle y | A | q \rangle \langle q | e_j \rangle dq dy \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_j \langle q | e_j \rangle \langle e_j | y \rangle \langle y | A | q \rangle dq dy \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \langle q | y \rangle \langle y | A | q \rangle dq dy \\ &= \int_{\mathbb{R}^n} \langle q | A | q \rangle dq \end{aligned}$$

where we have resolved the identity for first the $|e_j\rangle$'s and then the $|y\rangle$'s. Thus we are left with

$$\mathrm{tr}(A) = \int_{\mathbb{R}^n} \langle q | A | q \rangle dq. \quad (2.2.20)$$

Upon comparison with (2.1.9) we see that this is simply

$$\mathrm{tr}(A) = \int K_A(q, q) dq \quad (2.2.21)$$

as described. Then, using this we immediately have

$$\begin{aligned} \mathrm{tr}(A^\dagger A) &= \int_{\mathbb{R}^n} \langle q | A A^\dagger | q \rangle dq \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \langle q | A | y \rangle \langle y | A^\dagger | q \rangle dq dy \\ &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} |\langle q | A | y \rangle|^2 dq dy \\ &= \|K_A\|_{L^2}^2 = \|A\|_{HS}^2 \end{aligned}$$

where we have used (2.2.17) in the last equality. \square

Note then that this implies that the Hilbert-Schmidt norm for a trace class operator is given simply by the L^2 norm of the integral kernel.

Finally, we note the following Cauchy-Schwartz relation between the two classes:

Proposition 2.2.7. *If $A : E \rightarrow F$ and $B : F \rightarrow G$ are HS operators, then the product BA is of trace class and we have the Cauchy-Schwartz relation*

$$\|BA\|_{tr} \leq \|B\|_{HS} \|A\|_{HS}. \quad (2.2.22)$$

2.2.2 Statistical ensembles and density operators.

As mentioned previously, this section will be loosely based on the discussion in Section 4, Chapter 8 of [44]. Often in quantum mechanics we will wish to consider not just a system in a single quantum state, but a system in a *statistical ensemble* of quantum states. That is, we might wish to consider a system where we have imperfect information about what state the system is in but we know some statistical information about the states it could be in.

Given we are in such a situation, and we can describe the probability p_j that the system is occupying a quantum state $|\psi_j(t)\rangle$ at each instant, where $p_j \geq 0$ and $\sum_j p_j = 1$, we can define the *density operator* of a quantum state as follows.

Definition 2.2.8. For a set of orthonormal states on a Hilbert space $|\psi_j\rangle \in \mathcal{H}$ in a statistical ensemble with probabilities p_j s.t. $p_j \geq 0$, $\sum_j p_j = 1$, we define the density operator of the ensemble to be

$$\hat{\rho} = \sum_j p_j |\psi_j\rangle \langle \psi_j|. \quad (2.2.23)$$

Since our states $|\psi\rangle$ are taken to be normalized we have that

$$\begin{aligned} \text{tr}(\hat{\rho}) &= \sum_j \langle e_j | \hat{\rho} | e_j \rangle \\ &= \sum_j \sum_k p_k \langle e_j | \psi_k \rangle \langle \psi_k | e_j \rangle \\ &= \sum_k p_k \langle \psi_k | \left(\sum_j \langle e_j | e_j \rangle \right) | \psi_k \rangle \\ &= \sum_k p_k \langle \psi_k | \psi_k \rangle \\ &= 1. \end{aligned}$$

Clearly then $\hat{\rho}$ is a trace class operator since it has singular values given by $s_j(\hat{\rho}) = p_j$, and further than that it has trace 1. It is also self-adjoint and since the p_k 's are probabilities and hence are positive it is also positive semi-definite.

If we now wish to measure an observable \hat{A} in this ensemble, we simply find the expected value as the sum over the measurement of \hat{A} in the individual states multiplied by the probability. That is we take

$$\langle \hat{A} \rangle_{\text{ensemble}} = \sum_j p_j \langle \psi_j | \hat{A} | \psi_j \rangle. \quad (2.2.24)$$

Now by using the resolution of identity for an orthonormal basis $\{|e_k\rangle\}$ and rearranging, and then using our definition of the trace (2.2.7) we get that

$$\begin{aligned} \langle \hat{A} \rangle_{\text{ensemble}} &= \sum_j p_j \langle \psi_j | \hat{A} | \psi_j \rangle \\ &= \sum_j \sum_k p_j \langle \psi_j | e_k \rangle \langle e_k | \hat{A} | \psi_j \rangle \\ &= \sum_j \sum_k p_j \langle e_k | \hat{A} | \psi_j \rangle \langle \psi_j | e_k \rangle \\ &= \sum_k \langle e_k | \left(\hat{A} \sum_j p_j | \psi_j \rangle \langle \psi_j | \right) | e_k \rangle \\ &= \text{tr}(\hat{A} \hat{\rho}). \end{aligned}$$

Note that since we know that $\hat{\rho}$ is a trace-class operator, and our observable \hat{A} is a bounded operator, from (2.2.5) we know that this trace is well defined as $\hat{A}\hat{\rho}$ is of trace class.

Definition 2.2.9 (Purity of a quantum state). For $\hat{\rho}$ a density operator acting on a Hilbert space \mathcal{H} , we define the *purity of the quantum state* $\mu(\hat{\rho})$ to be the number

$$\mu(\hat{\rho}) = \text{tr}(\hat{\rho}^2). \quad (2.2.25)$$

The purity satisfies the relation

$$0 \leq \mu(\hat{\rho}) \leq 1 \quad (2.2.26)$$

and we say that a quantum state is pure if and only if its purity is exactly equal to 1.

Importantly, if a state is pure it means there exists a $\psi \in \mathcal{H}$ such that we can write the density operator associated to the state as

$$\hat{\rho} = |\psi\rangle \langle \psi|. \quad (2.2.27)$$

2.2.3 Time evolution of the density operator

If we consider a partially known quantum system evolving in time, we describe it by the state

$$|\psi(t)\rangle = \sum_j p_j |\psi_j(t)\rangle, \quad \sum_j p_j = 1, \quad p_j \geq 0 \quad (2.2.28)$$

where each individual state $|\psi_j(t)\rangle$ satisfies the same Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t} |\psi_j(t)\rangle = \hat{H} |\psi_j(t)\rangle, \quad (2.2.29)$$

where \hat{H} is the self-adjoint system Hamiltonian. If we let \hat{U}_t be the evolution operator resulting from the time evolution, i.e.

$$|\psi(t)\rangle = \hat{U}_t |\psi(0)\rangle \quad (2.2.30)$$

then clearly it is a unitary operator and satisfies the conjugated equations

$$i\hbar \frac{d}{dt} \hat{U}_t = \hat{H} \hat{U}_t, \quad i\hbar \frac{d}{dt} \hat{U}_t^\dagger = -\hat{U}_t^\dagger \hat{H}. \quad (2.2.31)$$

We then have the following well-known result for the time-evolution of the density operator.

Proposition 2.2.10 (The von Neumann equation). *Let $\hat{\rho}_0$ be the density operator of the mixed state (2.2.28) at time $t = 0$. At time t this density operator is given by*

$$\hat{\rho}_t = \hat{U}_t \hat{\rho}_0 \hat{U}_t^\dagger \quad (2.2.32)$$

and the mapping $t \rightarrow \hat{\rho}_t$ satisfies the operator evolution equation

$$i\hbar \frac{d}{dt} \hat{\rho}_t = [\hat{H}, \hat{\rho}_t] \quad (2.2.33)$$

which is known as the von Neumann equation.

Proof. The first part follows from the construction

$$\hat{\rho}_t = \sum_j p_j |\psi_j(t)\rangle \langle \psi_j(t)| = \sum_j p_j \hat{U}_t^\dagger |\psi_j(0)\rangle \langle \psi_j(0)| \hat{U}_t = \hat{U}_t^\dagger \hat{\rho}_0 \hat{U}_t. \quad (2.2.34)$$

For the Liouville-von Neumann equation itself, we differentiate (2.2.32) to get

$$\begin{aligned} i\hbar \frac{d}{dt} \hat{\rho}_t &= i\hbar \frac{d}{dt} (\hat{U}_t \hat{\rho}_0 \hat{U}_t^\dagger) \\ &= \hat{H} \hat{U}_t \hat{\rho}_0 \hat{U}_t^\dagger + \hat{U}_t \hat{\rho}_0 (-\hat{U}_t^\dagger) \hat{H} \\ &= \hat{H} \hat{\rho}_t - \hat{\rho}_t \hat{H} = [\hat{H}, \hat{\rho}_t]. \end{aligned}$$

□

2.2.4 Open quantum systems and the Lindblad equation

The standard theory we outlined in Section 2.2.3 is valid for a situation in which our quantum system does not interact with an environment, often referred to as a closed system. In reality though, all quantum systems interact with an environment in some form and we need to describe this open system in a suitable mathematically sound fashion. Here we will work towards justifying the use of the Lindblad equation [33][11] discussed in the introduction, which is the most general form of the Markovian master equation satisfying the so-called complete positivity condition, and can be viewed as the underlying equation describing the interaction of a quantum system with an environment.

The full proof that the Lindblad equation is the most general Markovian master equation satisfying complete positivity is involved and requires semigroup theory which will not be used elsewhere in this thesis. Because of this, we instead choose a more constructive heuristic approach to motivate its use. To do this we will first define complete positivity and then give a construction of the Lindblad equation starting from the classical Pauli master equation[40]. This section is based on the construction in the book “Quantum Dynamical Semigroups and Applications” by Alicki and Lendi [1] which also provides the complete proof based on semigroup theory.

Completely positive maps

If we have an open quantum system consisting of a system denoted by \mathcal{S} governed by internal dynamics and a reservoir \mathcal{R} which describes the external environment and interacts with the system, then we can write the Hilbert space governing the full internal and external systems as the tensor product of the Hilbert spaces governing the system and reservoir respectively. That is we write

$$\mathcal{H} = \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{R}}. \quad (2.2.35)$$

Using the notation we defined in (2.2.3) we let $\mathcal{T}(\mathcal{H}_{\mathcal{S}})$ the space of trace class operators acting on the Hilbert space $\mathcal{H}_{\mathcal{S}}$, and similarly by $\mathcal{B}(\mathcal{H}_{\mathcal{S}})$ the wider space of all linear and bounded operators. The subset of self-adjoint operators in $\mathcal{B}(\mathcal{H}_{\mathcal{S}})$ represent bounded observables and unbounded observables are treated as a limit of sequences of these bounded observables.

If we assume that we can prepare an initial state at $t_0 = 0$

$$\rho_0 \otimes \omega_{\mathcal{R}}, \quad (2.2.36)$$

where ρ_0 is the initial state of our internal system, and $\omega_{\mathcal{R}}$ is a fixed reference state of the environment, then we can use the time evolution (2.2.32) and the so called partial trace to write the evolved open system as the mapping

$$\Lambda_t : \mathcal{T}(\mathcal{H}_{\mathcal{S}}) \rightarrow \mathcal{T}(\mathcal{H}_{\mathcal{S}}) \quad (2.2.37)$$

defined by

$$\rho_t = \Lambda_t \rho_0 = \text{tr}_{\mathcal{R}} \left(U_t(\rho_0 \otimes \omega_{\mathcal{R}}) U_t^\dagger \right) \quad (2.2.38)$$

where U_t is the time evolution of $H = H_S \otimes H_R$.

The partial trace takes trace class operators on the full Hilbert space \mathcal{H} to trace class operators on the systems Hilbert space \mathcal{H}_S and is defined via

$$\langle \phi | \text{tr}_R \gamma | \psi \rangle = \sum_{\nu} \langle \phi \otimes e_{\nu} | \gamma | \psi \otimes e_{\nu} \rangle \quad (2.2.39)$$

where $\gamma \in \mathcal{T}(\mathcal{H}_S)$, ϕ and ψ are states in \mathcal{H}_S and $\{e_{\nu}\}$ form an arbitrary orthonormal basis of the reservoir.

If we now spectrally decompose our reservoir we can in fact characterize the class of maps Λ_t in terms of the system Hilbert space \mathcal{H}_S only. Namely, if we spectrally decompose

$$\omega_R = \sum_{\nu} \lambda_{\nu} |e_{\nu}\rangle \langle e_{\nu}| \quad (2.2.40)$$

and choose an orthonormal basis $\{s_k\}$ of \mathcal{H}_S then we can write the map Λ_t in (2.2.38) as the matrix

$$(\Lambda_t \rho)_{kl} = \sum_{\mu, \nu} \sum_{m, n} \lambda_{\nu} U_{\mu k, \nu m} \rho_{mn} \bar{U}_{\nu n, \mu l} \quad (2.2.41)$$

where

$$U_{\mu k, \nu m} = \langle s_k \otimes e_{\mu} | U | s_m \otimes e_{\nu} \rangle. \quad (2.2.42)$$

In particular then we can write the map Λ_t in the following standard form known as the *Kraus representation* (see for example [22] for a discussion of this):

$$\Lambda_t \rho = \sum_{\alpha} K_{\alpha} \rho K_{\alpha}^{\dagger} \quad (2.2.43)$$

where

$$K_{\alpha} \in \mathcal{B}(\mathcal{H}_S), \quad \sum_{\alpha} K_{\alpha}^{\dagger} K_{\alpha} = I, \quad (2.2.44)$$

I being the identity here. In terms of the U and λ , the operators K_{α} are given by

$$\{\alpha\} \equiv \{(\mu, \nu)\}, \quad (K_{\alpha})_{km} = \lambda_{\nu} U_{\mu k, \nu m}. \quad (2.2.45)$$

It turns out that maps of this form are the only viable candidates for irreversible time evolution of open quantum systems in the Schrödinger picture.

This can be seen by considering the conditions we wish such a map to satisfy if we want it to provide a valid description of the evolution of a density operator found as a subsystem of a system-environment system.

Firstly, we demand that the time evolution of the environment be *Markovian*. That is it has no memory-effects and can be treated basically as random noise. Without this the problem would not be tractable. In particular then, we require that

$$\Lambda_{t+s} = \Lambda_t \circ \Lambda_s. \quad (2.2.46)$$

Secondly, it must be trace preserving, otherwise the system may evolve to one with $\text{tr } \rho_t \neq 1$ which would violate the interpretation as a probabilistic ensemble.

Finally, we require that the evolved state ρ_t is positive, again for consistency with the interpretation as a probabilistic ensemble. However since we are dealing with a system coupled with an environment this is not so simple to state. There exists examples of pairs of operators ρ and σ which are themselves individually positive but whose tensor product $\rho \otimes \sigma$ is not positive. Hence we need a stronger condition than mere positivity of $\Lambda_t \rho$, this condition is known as *complete positivity*. For our purposes, this condition can be stated as follows:

Definition 2.2.11 (Complete Positivity). We say that the operator ρ_t is *completely positive* if and only if the product

$$\rho_t \otimes I_m, \quad m = 1, 2, \dots \quad (2.2.47)$$

is positive for all m .

The motivation behind this definition can be summarized as considering an m level system with Hamiltonian $H = 0$ placed far away from our open system. The combined system is then given by $\rho_t \otimes I_m$ and we require that this combination with a trivial system is positive for all m . This is a stronger condition than positivity and is called *complete positivity* and is enough to guarantee that the tensor product remains positive for more complicated combined systems.

It can be shown(see [1]) that completely positive maps can always be written in the form of (2.2.43) and hence this Kraus operator representation is the only form of maps we should consider when trying to describe time evolution of open quantum systems.

A constructive approach to the Lindblad equation

The *Pauli master equation*

$$\frac{d}{dt}p_j(t) = \sum_{k=1}^n (a_{jk}p_k(t) - a_{kj}p_j(t)), \quad k = 1, \dots, n \quad (2.2.48)$$

can be used to describe the probability that a state jumps from one discrete energy level to another. Here $a_{jk} \geq 0$ are the transition probabilities per unit time of jumping from the state j to the state k . These transition probabilities form matrices (a_{jk}) and (a_{kj}) which we call M and M^\dagger respectively. That is, we write

$$(Mx)_j = \sum_{k=1}^n a_{jk}x_k, \quad (M^\dagger x)_j = \sum_{k=1}^n a_{kj}x_k \quad (2.2.49)$$

where $x = (x_1, \dots, x_n)$.

Note that these are positive maps in the sense that for $x_k \geq 0$ we have $Mx, M^\dagger x \geq 0$. Using these maps we can rewrite the Pauli master equation (2.2.48) as a classical operator equation

$$\frac{d}{dt}p(t) = Mp(t) - (M^\dagger \mathbf{1}) \circ p(t) \quad (2.2.50)$$

where we have taken

$$p(t) = (p_1(t), p_2(t), \dots, p_n(t)), \quad \mathbb{1} = (1, 1, \dots, 1) \quad (2.2.51)$$

and

$$x \circ y = (x_1 y_1, x_2 y_2, \dots, x_n y_n) \quad (2.2.52)$$

denotes elementwise multiplication.

From here we now “quantize” (2.2.50). Quantizing is a topic we will cover in more detail in the next section of this background chapter from the point of view of semiclassical analysis, but for now we restrict ourselves to the following simple associative rules for quantization:

- We replace a probability distribution p with a density operator $\hat{\rho}$.
- We replace a positive transition map M with a completely positive quantum transition map $\hat{\Phi}$.
- We replace the product of two functions $x \circ y$ with a symmetric product of two operators $\hat{X} \circ \hat{Y} = \frac{1}{2}[\hat{X}, \hat{Y}]_+$.

where $[\hat{X}, \hat{Y}]_+ = \hat{X}\hat{Y} + \hat{Y}\hat{X}$ is the anticommutator.

We now extend our theory by introducing a Hamiltonian part (as well as an \hbar dependence to bring the equation in line with the von Neumann equation (2.2.33)) to the quantized version of equation (2.2.50)

$$\frac{\partial}{\partial t} \hat{\rho}_t = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_t] + \frac{1}{\hbar} \hat{\Phi} \hat{\rho}_t - \frac{1}{2\hbar} [\hat{\Phi}^\dagger(I), \hat{\rho}_t]_+. \quad (2.2.53)$$

Recalling that all completely positive maps can be written in the form $\hat{\Phi}\rho = \sum_\alpha \hat{L}_\alpha \rho \hat{L}_\alpha^\dagger$ we have

$$\begin{aligned} \frac{\partial}{\partial t} \hat{\rho}_t &= -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_t] + \frac{1}{\hbar} \hat{\Phi} \hat{\rho}_t - \frac{1}{2\hbar} \hat{\Phi}^\dagger(I) \hat{\rho}_t - \hat{\rho}_t \hat{\Phi}^\dagger(I) \\ &= -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_t] + \frac{1}{\hbar} \sum_j \hat{L}_j \hat{\rho}_t \hat{L}_j^\dagger - \frac{1}{2\hbar} \sum_j \left(\hat{L}_j^\dagger \hat{L}_j \hat{\rho}_t + \hat{\rho}_t \hat{L}_j^\dagger \hat{L}_j \right) \\ &= -\frac{i}{\hbar} [\hat{H}, \hat{\rho}_t] + \frac{1}{2\hbar} \sum_j 2\hat{L}_j \hat{\rho}_t \hat{L}_j^\dagger - \hat{L}_j^\dagger \hat{L}_j \hat{\rho}_t - \hat{\rho}_t \hat{L}_j^\dagger \hat{L}_j. \end{aligned}$$

Hence, combining terms into commutators and dropping the explicit t dependence from the notation, we arrive at the following general form of the Lindblad equation, the most general Markovian master equation satisfying the complete positivity condition:

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \frac{1}{2\hbar} \sum_j [\hat{L}_j \hat{\rho}, \hat{L}_j^\dagger] - [\hat{\rho} \hat{L}_j^\dagger, \hat{L}_j]. \quad (2.2.54)$$

Lindblad showed that this equation, or more precisely the generator, is the most general equation for any separable Hilbert space for countable sets of indices $\{j\}$ and

$\hat{H}, \sum_j \hat{L}_j^\dagger \hat{L}_j \in \mathcal{B}(\mathcal{H}_S)$ [33]. Separately, Gorini, Kossakowski and Sudarshan showed a similar result for the generator of a quantum dynamical semigroup in the case of a finite dimensional Hilbert space \mathcal{H}_S [11].

Here the \hat{L}_j 's are known as the Lindblad operators and need to be determined from the system and environment we are studying. The above construction gives an idea of how you can do this by decomposing your system into elementary transition maps $\hat{\rho} \mapsto \hat{L}_j \hat{\rho} \hat{L}_j^\dagger$ each of which describe independent irreversible processes. This can be quite involved and relies on for instance symmetry properties of the system as well as other known properties but can be used to guess a relevant form of the transition map Φ .

2.2.5 Examples of Lindblad equations

In this section we will, following [22], give some brief examples of basic Lindblad equations for some simple open systems.

Dephasing

We start with possibly the simplest choice of Lindblad operators we could make, a single operator proportional to the internal Hamiltonian of the system. That is we take

$$\hat{L} = \sqrt{\gamma} \hat{H}. \quad (2.2.55)$$

In this case, the Lindblad equation (2.2.54) reduces to

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \frac{\gamma}{\hbar} \left(\hat{H} \hat{\rho} \hat{H} - \frac{1}{2} \hat{H}^2 \hat{\rho} - \frac{1}{2} \hat{\rho} \hat{H}^2 \right). \quad (2.2.56)$$

The effect of the environment is just a multiple of the Hamiltonian, and hence commutes with it. As a result, the system exchanges no energy with the environment and vice-versa, the resulting evolution being purely dephasing. This is in contrast to more complicated choices of environment where we might see a change due to the loss of energy to the environment. The dephasing case is discussed in much more detail for the case of qubits in [22]. Here we simply note that the dephasing Lindblad equation (2.2.56) can be solved exactly in the energy eigenbasis $\hat{H} = \sum_m E_m |m\rangle \langle m|$ by

$$\rho_{mn}(t) = \langle m | \hat{\rho} | n \rangle = \rho_{mn}(0) \exp \left(-\frac{i}{\hbar} (E_m - E_n) t - \frac{\gamma}{2\hbar} (E_m - E_n)^2 t \right). \quad (2.2.57)$$

Importantly, the energy eigenstates remain unaffected by the environment and we see exponential decay of the cross terms (i.e. $m \neq n$), which correspond to the quantum coherences, from the environmental effects. The factor $\gamma > 0$ governs the rate of this decay. In [22] a more in depth study of the dephasing of qubits is given and upon comparison with this study it is apparent that γ is proportional to the temperature of the dephasing environment.

Damping of a Harmonic Oscillator

We restrict ourselves to the case of a harmonic oscillator Hamiltonian given by

$$\hat{H} = \hbar\omega\hat{a}^\dagger\hat{a} \quad (2.2.58)$$

where \hat{a}^\dagger and \hat{a} are the usual ladder or creation/annihilation operators and ω is the harmonic oscillator frequency. If we now choose $\hat{L} = \sqrt{\hbar\mu}\hat{a}$ we have the Lindblad equation

$$\frac{\partial\hat{\rho}}{\partial t} = -i\omega[\hat{a}^\dagger\hat{a}, \hat{\rho}] + \mu \left(\hat{a}\hat{\rho}\hat{a}^\dagger - \frac{1}{2}\hat{a}^\dagger\hat{a}\hat{\rho} - \frac{1}{2}\hat{\rho}\hat{a}^\dagger\hat{a} \right). \quad (2.2.59)$$

We see that this situation is almost directly equivalent to that described by the Pauli master equation (2.2.48) where instead of transition probabilities we have the ladder operator \hat{a} .

If as an initial state $\hat{\rho}_0$ we choose a pure coherent state density operator (we will discuss these in more detail later on in section 2.7) of the form

$$\begin{aligned} \hat{\rho}_0 &= |\alpha_0\rangle \langle \alpha_0| \\ &= e^{-|\alpha_0|^2} \exp(\alpha_0\hat{a}^\dagger) |0\rangle \langle 0| \exp(\alpha_0^*\hat{a}) \end{aligned} \quad (2.2.60)$$

where

$$|\alpha_0\rangle = \exp(\alpha_0\hat{a}^\dagger - \alpha_0^*\hat{a}) |0\rangle \quad (2.2.61)$$

for $|0\rangle$ the ground state and α_0 a complex number, the solution to the Lindblad equation (2.2.59) is simply

$$\hat{\rho}_t = |\alpha_t\rangle \langle \alpha_t| \quad (2.2.62)$$

in the same form as above with

$$\alpha_t = \alpha_0 \exp\left(-i\omega t - \frac{\mu}{2}t\right). \quad (2.2.63)$$

Importantly then, the time evolution maintains the purity of the initial state and describes the coherent state spiralling towards the origin, in the $t \rightarrow \infty$ limit reaching the ground state. The quantity μ is the dissipation rate of the energy of the system as can be seen by considering the expectation value of the energy:

$$\langle \alpha_t | H | \alpha_t \rangle = e^{-\mu t} \langle \alpha_0 | H | \alpha_0 \rangle. \quad (2.2.64)$$

If we now consider a cat state, i.e. a superposition of two coherent states

$$|\psi_0\rangle = \frac{1}{\sqrt{\mathcal{N}}} (|\alpha_0\rangle + |\beta_0\rangle) \quad (2.2.65)$$

and we separate the states $|\alpha_0\rangle$ and $|\beta_0\rangle$ in phase space such that the separation $|\alpha_0 - \beta_0|$ is large compared to the scale of the quantum uncertainties, then the initial density operator is given by

$$\hat{\rho}_0 = \frac{1}{\mathcal{N}} \left(|\alpha_0\rangle \langle \alpha_0| + |\beta_0\rangle \langle \beta_0| + |\alpha_0\rangle \langle \beta_0| + |\beta_0\rangle \langle \alpha_0| \right). \quad (2.2.66)$$

The ansatz

$$\hat{\rho}_t = \frac{1}{\mathcal{N}} \left(|\alpha_t\rangle \langle \alpha_t| + |\beta_t\rangle \langle \beta_t| + c_t |\alpha_t\rangle \langle \beta_t| + c_t^* |\beta_t\rangle \langle \alpha_t| \right) \quad (2.2.67)$$

can be shown to solve the Lindblad equation in this case if the prefactor c_t is given by

$$c_t = c_0 \exp \left(\left[-\frac{1}{2} |\alpha_0 - \beta_0|^2 + i \operatorname{Im}(\alpha_0 \beta_0^*) \right] (1 - e^{-\mu t}) \right). \quad (2.2.68)$$

Hence the diagonal terms evolve as in the case of a single state, while the cross terms experience an additional suppression which for short time scales (that is short compared to the dissipative timescale $t \ll 1/\mu$) is approximated by an exponential decay

$$|c_t| = |c_0| \exp \left(-\frac{\mu}{2} |\alpha_0 - \beta_0|^2 t \right) \quad (2.2.69)$$

which can be seen simply by expanding the exponential. Hence as the distance between the states increased, the rate of this suppression increases and the quantity

$$\mu_{\text{deco}} = \frac{\gamma}{2} |\alpha_0 - \beta_0|^2 \quad (2.2.70)$$

is known as the *decoherence rate* of the system. We will discuss decoherence in more detail later in this chapter but for now simply note that this is extremely fast acting as the distance $|\alpha_0 - \beta_0|$ increases.

A Harmonic Oscillator Coupled to a Heat Bath

A very common model of the environment is a so called “heat bath” environment[1], consisting of a damping or friction force decreasing the energy of the system as well as a Langevin force pumping energy into the system. This is very similar to the previous example, though now we have a second Lindblad operator a^\dagger . In particular, take

$$\hat{L}_1 = \mu \hat{a}, \quad \hat{L}_2 = \gamma \hat{a}^\dagger \quad (2.2.71)$$

where μ is the dissipation rate and γ can be thought of as similarly the rate of energy being pumped into the system.

This leads to the following Lindblad equation in the case of the harmonic oscillator Hamiltonian $\hat{H} = \omega \hat{a}^\dagger \hat{a}$

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} \omega [\hat{a}^\dagger \hat{a}, \hat{\rho}] + \frac{1}{2\hbar} \mu \left([\hat{a} \hat{\rho}, \hat{a}^\dagger] + [\hat{a}, \hat{\rho} \hat{a}^\dagger] \right) + \frac{1}{2\hbar} \gamma \left([\hat{a}^\dagger \hat{\rho}, \hat{a}] + [\hat{a}^\dagger, \hat{\rho} \hat{a}] \right). \quad (2.2.72)$$

If we assume that the rate of energy pumped into the system is lower than the dissipation rate, that is $\gamma < \mu$, then it can be shown (see [1]), that the temperature of the system β is given by

$$\beta = \frac{1}{\hbar \omega} \ln \left(\frac{\mu}{\gamma} \right). \quad (2.2.73)$$

A Random Scatterer

If we take as our Lindblad operators a single operator $L = \sqrt{\sigma}\hat{q}$ then this corresponds to an environment described by random scattering off of a cloud or gas of dust particles. In this case the Lindblad equation is given by

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{H}, \hat{\rho}] + \frac{\sigma}{2\hbar} (2\hat{q}\hat{\rho}\hat{q} - \hat{q}^2\hat{\rho} - \hat{\rho}\hat{q}^2). \quad (2.2.74)$$

This type of environment is one of the simplest we can choose and has been used very commonly to investigate decoherence, see for instance [25] which among other things gives a table of physically realistic values for the parameter σ as well as similar weights for other common Lindblad descriptions of the environment. We will study the scattering case and how it relates to decoherence in greater detail in the next chapter.

2.3 Symplectic geometry

Before going any further we introduce some basic symplectic geometry theory. This will be based primarily on [2]. We start by motivating the interest of symplectic geometry from the viewpoint of classical Hamiltonian dynamics.

2.3.1 Hamiltonian dynamics

Recall that for position coordinates $q = (q_1, q_2, \dots, q_n)$ and momentum coordinates $p = (p_1, p_2, \dots, p_n)$ the time evolution of a system is described by *Hamilton's equations* which can be written as

$$\frac{d}{dt}q = \frac{\partial H}{\partial p}, \quad \frac{d}{dt}p = -\frac{\partial H}{\partial q} \quad (2.3.1)$$

where H is the *Hamiltonian* of the system often written as $H = H(q, p, t) = T + V$ where T is the kinetic energy of the system and V is the potential energy of the system, given as functions of q and p .

We define the Poisson bracket as

$$\{f, g\} := \sum_j \frac{\partial f}{\partial q_j} \frac{\partial g}{\partial p_j} - \frac{\partial f}{\partial p_j} \frac{\partial g}{\partial q_j} \quad (2.3.2)$$

for suitably differentiable functions f and g . Using this we can write Hamilton's equations as

$$\frac{d}{dt}q = \{q, H\}, \quad \frac{d}{dt}p = \{p, H\} \quad (2.3.3)$$

and this evolution must hold for more general observables of the system $f(q, p, t)$

$$\frac{d}{dt}f = \{f, H\}, \quad (2.3.4)$$

this is known as the *Liouville Equation*.

2.3.2 Linear symplectic maps

We start by describing symplectic vector spaces. Let V be a vector space over the field K .

Definition 2.3.1 (Symplectic form and symplectic vector spaces). A symplectic form is a bilinear map

$$\omega : V \times V \rightarrow K \quad (2.3.5)$$

that satisfies

$$\omega(v, w) = -\omega(w, v) \quad \forall v, w \in V, \quad (2.3.6)$$

and

$$\omega(v, w) = 0 \quad \forall v \in V \quad (2.3.7)$$

only if $w = 0$.

The vector space V is called a *symplectic vector space* if it is equipped with such a form. We say that two vectors in V are *skew-orthogonal* if $\omega(v, w) = 0$.

For $V = K^{2n}$, the standard symplectic form is given by

$$\omega(v, w) = v \cdot \Omega w \quad (2.3.8)$$

where we have in block form

$$\Omega = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \quad (2.3.9)$$

for I_n the $n \times n$ identity matrix with v and w column vectors.

Now, let W be an n -dimensional vector space over K and W^* be its dual space, then the space $V = W \oplus W^*$ is a symplectic space equipped with the form $\omega : V \times V \rightarrow K$ such that

$$\omega(v_1 + \chi_1, v_2 + \chi_2) = \chi_1(v_2) - \chi_2(v_1) \quad (2.3.10)$$

for $v_1, v_2 \in W$ and $\chi_1, \chi_2 \in W^*$.

How can we relate this back to Hamiltonian systems? We start by noting that, taking $x = (q, p)$ a point in phase space, we can write Hamilton's equations directly as

$$\frac{d}{dt}x = \Omega \nabla H(x) \quad (2.3.11)$$

where $\nabla = (\partial_q, \partial_p)$ is the phase-space gradient, Ω is the standard symplectic matrix above and $H(x)$ is the Hamiltonian of our system as a function of x .

Note as well that the equation for the evolution of an observable f (2.3.4), and indeed a poisson bracket in general, can be written in the following form:

$$\frac{d}{dt}f = \nabla f \cdot \Omega \nabla H \quad (2.3.12)$$

or, more directly in terms of the symplectic form ω

$$\frac{d}{dt}f = \omega(\nabla f, \nabla H). \quad (2.3.13)$$

Hence, Hamiltonian dynamics are naturally symplectic.

Definition 2.3.2 (Symplectic maps). Let V_i , $i = 1, 2$ be two symplectic vector spaces equipped with symplectic forms ω_i and take $\phi : V_1 \rightarrow V_2$ to be a linear map, then if

$$\omega_2(\phi(v), \phi(w)) = \omega_1(v, w), \quad \forall v, w \in V_1 \quad (2.3.14)$$

then we call ϕ a *symplectic map*.

Note that all symplectic maps are necessarily injective due to the non-degeneracy of ω and if the dimensions of the two spaces are the same (and non-infinite) then ϕ must be an isomorphism which we will call a *symplectomorphism*.

If $(V_1, \omega_1) = (V_2, \omega_2) = (V, \omega)$ then ϕ must be an automorphism. The symplectic automorphisms form a group called the *symplectic group* and this is denoted by $Sp(V)$ in the general case and by $Sp_n(K)$ ¹ in the case that the vector space V is given by simply K^{2n} .

Elements of $Sp_n(K)$ are matrices from GL_{2n} , the group of $2n \times 2n$ invertible matrices equipped with ordinary matrix multiplication. If we take as our element $M \in Sp_n(K)$ and the standard form of ω

$$\omega(v, w) = v \cdot \Omega w \quad (2.3.15)$$

we see that a matrix that leaves this form invariant, that is

$$\omega(Mv, Mw) = \omega(v, w) \quad (2.3.16)$$

satisfies

$$M^T \Omega M = \Omega. \quad (2.3.17)$$

The identity matrix I and Ω itself clearly satisfy (2.3.17). We note the following equivalent conditions which are found by applying the condition (2.3.17):

•

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \in Sp_n(K), \quad (2.3.18)$$

•

$$A^T C = C^T A, B^T D = D^T B, A^T D - C^T B = I, \quad (2.3.19)$$

•

$$AB^T = BA^T, CD^T = DC^T, AD^T - BC^T = I. \quad (2.3.20)$$

Some special symplectic matrices are the matrix

$$U_A = \begin{pmatrix} A & 0 \\ 0 & (A^T)^{-1} \end{pmatrix} \quad (2.3.21)$$

and the matrix

$$T_B = \begin{pmatrix} I & B \\ 0 & I \end{pmatrix} \quad (2.3.22)$$

¹sometimes $Sp_{2n}(K)$ in the literature

where $B = B^T$. These matrices along with the standard form Ω generate the group $Sp_n(K)[9]$. Since they generate the group and all of the matrices have determinant 1, we have that

$$\det M = 1 \quad \text{for } M \in Sp_n(K). \quad (2.3.23)$$

Finally we note that if M has an eigenvalue λ with multiplicity k , then the inverse $1/\lambda$ is also an eigenvalue with multiplicity k .

2.3.3 Quadratic Hamiltonian systems

If we return to Hamiltonian systems and we take our Hamiltonian $H(x)$ to be quadratic, that is we have

$$H(x) = \frac{1}{2}x \cdot Qx \quad (2.3.24)$$

for a symmetric matrix Q then we immediately have $\nabla H(x) = Qx$ and hence (2.3.11) becomes

$$\frac{d}{dt}x = \Omega Qx = Fx \quad (2.3.25)$$

where we have defined $F = \Omega Q$ which is often known as the *Hamiltonian map*. In this case we can solve this first order equation directly to see that the phase space trajectories are determined by

$$x(t) = e^{tF}x_0 = S(t)x_0 \quad (2.3.26)$$

for an initial condition x_0 and $S(t) := e^{tF}$. The matrix $S(t)$ is a symplectic matrix. This can be seen simply by checking the condition (2.3.17). At $t = 0$ this clearly holds and we see that

$$\frac{d}{dt}(S^T(t)\Omega S(t)) = S^T(t)(F^T\Omega + \Omega F)S(t) = 0 \quad (2.3.27)$$

by using our definition of $F = \Omega Q$ and the fact that Q is symmetric. Hence, integrating we have $S^T(t)\Omega S(t) = \Omega$ and thus $S(t)$ is symplectic for all t .

There is a lot more that could be said about the symplectic structure of Hamiltonian dynamics, and we will touch on some of these in later chapters, but for now we simply give the basic motivation. A more detailed description of the symplectic theory of Hamiltonian systems is given in chapter 3 of [2].

2.3.4 Lagrangian subspaces and complex structures

Let W be a linear subspace of the $2n$ dimensional symplectic space (V, ω) with $\dim W = k$. We define

$$W^\omega := \{v \in V \mid \omega(v, w) = 0 \quad \forall w \in W\} \quad (2.3.28)$$

to be the *skew-orthogonal* space of W which has dimension

$$\dim W^\omega = \dim V - \dim W = 2n - k. \quad (2.3.29)$$

We now introduce the most important subspaces of a symplectic space (V, ω) quoted from [2]:

Definition 2.3.3 (Symplectic subspaces [2]). We say

- (i) A subspace Q of V with $\omega|_Q = 0$ is an *isotropic* subspace of (V, ω) .
- (ii) A subspace $W \subset V$ with $\omega|_W$ non-degenerate is called a *symplectic subspace*
- (iii) A subspace $W \subset V$ with W^ω isotropic is called *co-isotropic*
- (iv) A subspace $L \subset V$ which is isotropic and co-isotropic, hence $L^\perp = L$ is called a *Lagrangian* subspace.

For a subspace $W \subset V$ with $\dim W = k$ we have the following results

$$\begin{aligned} W \text{ isotropic} &\iff W \subset W^\omega \Rightarrow k \leq n, \\ W \text{ co-isotropic} &\iff W \supset W^\omega \Rightarrow k \geq n, \\ W \text{ Lagrangian} &\iff W = W^\omega \Rightarrow k = n. \end{aligned}$$

Thus we can describe a Lagrangian subspace as a *maximally isotropic* subspace.

Complex structures

We now introduce the idea of equipping a symplectic space with a complex structure. So far we have considered the space \mathbb{R}^{2n} equipped with the canonical Euclidean structure of the dot product

$$s(v, w) := \langle v, w \rangle = v \cdot w = v^T w = \sum_{j=1}^{2n} v_j w_j \quad (2.3.30)$$

where we treat $v, w \in \mathbb{R}^{2n}$ as column vectors, as well as the canonical symplectic structure

$$\omega(v, w) = v \cdot \Omega w = v^T \Omega w = \sum_{i=1}^n (v_i w_{n+i} - v_{n+i} w_i). \quad (2.3.31)$$

We can identify $\mathbb{R}^{2n} \simeq \mathbb{C}$ by

$$v = \begin{pmatrix} x \\ p \end{pmatrix} \leftrightarrow z = x + ip \quad (2.3.32)$$

and then the operation iz corresponds to the operation

$$v \mapsto -\Omega v = \begin{pmatrix} -p \\ x \end{pmatrix}. \quad (2.3.33)$$

This operation

$$\Omega : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n} \quad (2.3.34)$$

where $\Omega^2 = -I$ supplies \mathbb{R}^{2n} with a *complex structure*.

Definition 2.3.4. Let V be a vector space over the field \mathbb{R} . A linear map $J : V \rightarrow V$ is called a *complex structure* if and only if

$$J^2 = -I_V \quad (2.3.35)$$

where I_V is the identity on V .

If V is also a symplectic vector space with symplectic form ω , we say that J is *compatible* with ω if

$$\omega(Jv, Jw) = \omega(v, w) \quad \forall v, w \in V. \quad (2.3.36)$$

A vector space V with an arbitrary complex structure J can be made into a complex vector space, i.e. a space over the field \mathbb{C} rather than \mathbb{R} , via the identification

$$iv := Jv. \quad (2.3.37)$$

If we consider the *complexification* of V defined by

$$V_c := V \otimes_{\mathbb{R}} \mathbb{C} \quad (2.3.38)$$

we can extend J linearly and then J has the eigenvalues $\pm i$. The eigenspaces are n -dimensional and given by

$$V_c^+ := \{v - iJv, v \in V\}, \quad \bar{V}_c^+ := \{v + iJv, v \in V\}, \quad (2.3.39)$$

and we have that

$$V_c = V_c^+ \oplus \bar{V}_c^+ \quad (2.3.40)$$

and

$$v \mapsto v - iJv \quad (2.3.41)$$

defines a complex vector space isomorphism between the (V, J) and (V_c^+, i) .

When J is a complex structure compatible with the symplectic form ω we define

$$g(v, w) := \omega(v, Jw), \quad v, w \in V \quad (2.3.42)$$

which since it is compatible implies

$$g(Jv, w) = \omega(v, w). \quad (2.3.43)$$

Since $J^2 = -1$ and ω is skew-symmetric, we have that

$$g(v, w) = g(w, v) \quad (2.3.44)$$

and

$$g(Jv, Jw) = g(v, w). \quad (2.3.45)$$

Thus g is a symmetric, non-degenerate bilinear form which we call a ω -*compatible pseudohermitian metric*.

When $g(v, v) \geq 0 \quad \forall v \in V$ we call g a Hermitian metric, J a positive compatible complex structure and the triple (V, ω, J) a *Kähler vector space*.

Theorem 2.3.5 (Equipping a space with a complex structure[2]). *Every symplectic vector space (V, ω) can be given a compatible positive complex structure J and a Hermitian structure g .*

Remark 2.3.6. An analagous statement holds for Hilbert spaces with a skew-symmetric weakly non-degenerate bilinear form ω .

2.4 Translation operators

We will wish to define the concept of a Gaussian coherent state later and these are often defined as linear translations of the ground state of the harmonic oscillator. To complete this definition we will need to introduce the concept of the Weyl-Heisenberg translation operators. These operators are extremely useful and we will see that it also allows us to define the characteristic function of our system very simply so it is worth spending some time on it now. As well as this, it can be used to relate the Weyl quantization and the Fourier transform as we will see. In the following discussion we will broadly follow the opening pages of the book “Coherent states and Applications in Mathematical Physics” by Monique Combescure and Didier Robert [5].

As before, we assume we are working with n -dimensional quantum mechanics with our Hilbert space $\mathcal{H} = L^2(\mathbb{R}^n)$ with the usual self-adjoint position and momentum operators

$$\hat{q} = (\hat{q}_1, \dots, \hat{q}_n) \quad (2.4.1)$$

and

$$\hat{p} = (\hat{p}_1, \dots, \hat{p}_n) \quad (2.4.2)$$

where

$$\hat{p}_j = -i\hbar \frac{\partial}{\partial q_j}. \quad (2.4.3)$$

These operators obey the standard Heisenberg commutation relations

$$[\hat{p}_j, \hat{q}_j] = -i\hbar \delta_{ij} \quad (2.4.4)$$

and

$$[\hat{q}_i, \hat{q}_j] = 0, \quad [\hat{p}_i, \hat{p}_j] = 0. \quad (2.4.5)$$

The operator $p \cdot \hat{q} - q \cdot \hat{p}$ is well defined for $x = (q, p) \in \mathbb{R}^{2n}$. This operator is self-adjoint and hence generates the following unitary operator which is known as the *twisted* Weyl-Heisenberg translation operator:

$$\hat{T}_\Omega(x) = \exp\left(\frac{i}{\hbar}(p \cdot \hat{q} - q \cdot \hat{p})\right) = \exp\left(-\frac{i}{\hbar}x \cdot \Omega \hat{x}\right), \quad (2.4.6)$$

where $\hat{x} = (\hat{q}, \hat{p})$. This is in contrast to the standard Weyl-Heisenberg operator:

$$\hat{T}(x) = \exp\left(-\frac{i}{\hbar}x \cdot \hat{x}\right). \quad (2.4.7)$$

Here $\Omega = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$ is the standard symplectic matrix we discussed earlier (2.3.9). Note that

$$\hat{T}_\Omega(x) = \hat{T}(\Omega^T x), \quad \text{and} \quad \hat{T}(x) = \hat{T}_\Omega(\Omega x). \quad (2.4.8)$$

The multiplication law for these operators can be found using the famous Baker-Campbell-Hausdorff result (with some restricting assumptions that simplify things). Let's briefly recall this result and the assumptions needed:

Lemma 2.4.1 (A Simple Baker-Campbell-Hausdorff result). *For two self adjoint operators \hat{A}, \hat{B} in a Hilbert space \mathcal{H} we have*

$$\exp(\hat{A} + \hat{B}) = \exp\left(-\frac{1}{2}[\hat{A}, \hat{B}]\right) \exp(\hat{A}) \exp(\hat{B}) \quad (2.4.9)$$

under the following assumptions:

- (i) There exists a linear subspace \mathcal{H}_0 dense in \mathcal{H}
- (ii) \mathcal{H}_0 is invariant for $\hat{A}, \hat{B}, e^{t\hat{A}}, e^{t\hat{B}}$ for all $t \in \mathbb{R}$
- (iii) \hat{A} and \hat{B} commute with $[\hat{A}, \hat{B}]$ and $i[\hat{A}, \hat{B}]$

Proof. We can prove this straightforwardly as follows. Let

$$F(t)u = e^{-\frac{t^2}{2}[\hat{A}, \hat{B}]} e^{t\hat{A}} e^{t\hat{B}} u \quad (2.4.10)$$

for a fixed $u \in \mathcal{H}_0$ and take the derivative with respect to t to get

$$F'(t)u = -t[\hat{A}, \hat{B}]e^{-\frac{t^2}{2}[\hat{A}, \hat{B}]} e^{t\hat{A}} e^{t\hat{B}} u + e^{-\frac{t^2}{2}[\hat{A}, \hat{B}]} e^{t\hat{A}} (\hat{A} + \hat{B}) e^{t\hat{B}} u \quad (2.4.11)$$

We can commute the \hat{A} to the left directly, thanks to our commutation assumptions, but we need to be careful commuting the \hat{B} to the left since it does not commute with $e^{t\hat{A}}$.

Note that

$$\frac{d}{dt} \left(e^{t\hat{A}} \hat{B} e^{-t\hat{A}} \right) = e^{t\hat{A}} [\hat{A}, \hat{B}] e^{-t\hat{A}} = [\hat{A}, \hat{B}] \quad (2.4.12)$$

since everything in the last equality commutes. Thus,

$$e^{t\hat{A}} \hat{B} e^{-t\hat{A}} = t[\hat{A}, \hat{B}] + \hat{B} \quad (2.4.13)$$

and hence

$$e^{t\hat{A}} \hat{B} = t[\hat{A}, \hat{B}] e^{t\hat{A}} + \hat{B} e^{t\hat{A}}. \quad (2.4.14)$$

Using this to commute everything to the left in (2.4.11) and cancelling terms we arrive at

$$F'(t)u = (\hat{A} + \hat{B})F(t)u \quad (2.4.15)$$

and as a result

$$F(t) = \exp(t(\hat{A} + \hat{B})). \quad (2.4.16)$$

The choice $t = 1$ then gives the result. \square

A good choice of \mathcal{H}_0 is the Schwartz space (more on this later) and applying this we get the following multiplication law for the translation operators:

Lemma 2.4.2 (A multiplication law for the translation operators).

$$\hat{T}_\Omega(x)\hat{T}_\Omega(x') = \exp\left(-\frac{i}{2\hbar}\omega(x, x')\right)\hat{T}_\Omega(x+x') \quad (2.4.17)$$

where $x = (q, p), x' = (q', p')$. Note that this implies

$$\hat{T}_\Omega(x)\hat{T}_\Omega(x') = \exp\left(-\frac{i}{\hbar}\omega(x, x')\right)\hat{T}_\Omega(x')\hat{T}_\Omega(x) \quad (2.4.18)$$

and in particular

$$\left(\hat{T}_\Omega(x)\right)^{-1} = \left(\hat{T}_\Omega(x)\right)^* = \hat{T}_\Omega(-x). \quad (2.4.19)$$

Proof. Let $\hat{A} = \frac{i}{\hbar}x \cdot \Omega\hat{x}$ and $\hat{B} = \frac{i}{\hbar}x' \cdot \Omega\hat{x}$, i.e. the exponents of our two translation operators. Then using (2.4.1) we have that

$$\hat{T}_\Omega(x)\hat{T}_\Omega(x') = \exp(\hat{A})\exp(\hat{B}) = \exp\left(\frac{1}{2}[\hat{A}, \hat{B}]\right)\exp(\hat{A} + \hat{B}). \quad (2.4.20)$$

We can see straight away that

$$\exp(\hat{A} + \hat{B}) = \exp\left(\frac{i}{\hbar}(x+x') \cdot \Omega\hat{x}\right) = \hat{T}_\Omega(x+x'). \quad (2.4.21)$$

For the prefactor, we expand out the commutator and write it in terms of commutators of \hat{p} and \hat{q} :

$$[\hat{A}, \hat{B}] = \left(\frac{i}{\hbar}\right)^2 ([p \cdot \hat{q}, p' \cdot \hat{q}] - [p \cdot \hat{q}, q' \cdot \hat{p}] - [q \cdot \hat{p}, p' \cdot \hat{q}] + [q \cdot \hat{p}, q' \cdot \hat{p}]). \quad (2.4.22)$$

Recalling that for vectors a, c and vector operators \hat{b}, \hat{d} that we have

$$[a \cdot \hat{b}, c \cdot \hat{d}] = \sum_{jk} [a_j \hat{b}_j, c_k \hat{d}_k] = \sum_{jk} a_j [\hat{b}_j, \hat{d}_k] c_k \quad (2.4.23)$$

and recalling our commutation relations (2.4.4), (2.4.5) we see that

$$\begin{aligned} [\hat{A}, \hat{B}] &= \left(\frac{i}{\hbar}\right)^2 (0 - i\hbar p \cdot q' + i\hbar q \cdot p' + 0) \\ &= \frac{i}{\hbar}(p \cdot q' - q \cdot p') \\ &= -\frac{i}{\hbar}\omega(x, x') \end{aligned} \quad (2.4.24)$$

and hence

$$\hat{T}_\Omega(x)\hat{T}_\Omega(x') = \exp\left(-\frac{i}{2\hbar}\omega(x, x')\right)\hat{T}_\Omega(x+x'). \quad (2.4.25)$$

For (2.4.18) simply note that swapping the order of x, x' swaps the sign of $\frac{i}{2\hbar}\omega(x, x')$ and to prove (2.4.19) simply use (2.4.17) with $x' = -x$. \square

Now note the following property:

$$\hat{T}_\Omega(x) \begin{pmatrix} \hat{q} \\ \hat{p} \end{pmatrix} \hat{T}_\Omega(x)^{-1} = \begin{pmatrix} \hat{q} - q \\ \hat{p} - p \end{pmatrix} \quad (2.4.26)$$

We can prove this quickly by first noting that

$$i\hbar \frac{d}{dt} \hat{T}_\Omega(tx) = -x \cdot \Omega \hat{x} \hat{T}_\Omega(tx) \quad (2.4.27)$$

and hence

$$i\hbar \frac{d}{dt} \left(\hat{T}_\Omega(tx) \hat{q} \hat{T}_\Omega(-tx) \right) = \hat{T}_\Omega(tx) [\hat{q}, p \cdot \hat{q} - q \cdot \hat{p}] \hat{T}_\Omega(-tx). \quad (2.4.28)$$

Because $[\hat{q}, p \cdot \hat{q} - q \cdot \hat{p}] = -i\hbar q$ we get the result via existence and uniqueness of solutions to ODEs since $\hat{q} - tq$ satisfies the same ODE. The same argument works for \hat{p} . From this it is not hard to see why these operators are known as translation operators.

Corollary 2.4.3.

$$\hat{T}_\Omega(x) = e^{-\frac{i}{2\hbar} q \cdot p} e^{\frac{i}{\hbar} p \cdot \hat{q}} e^{-\frac{i}{\hbar} q \cdot \hat{p}} \quad (2.4.29)$$

Proof. This can be seen as a direct result of (2.4.17) with the choice $x_1 = (0, p)$ and $x_2 = (q, 0)$. Then

$$\begin{aligned} \hat{T}_\Omega(x) &= \hat{T}_\Omega(x_1 + x_2) \\ &= \exp \left(\frac{i}{2\hbar} \omega(x_1, x_2) \right) \hat{T}_\Omega(x_1) \hat{T}_\Omega(x_2) \\ &= e^{-\frac{i}{2\hbar} q \cdot p} e^{\frac{i}{\hbar} p \cdot \hat{q}} e^{-\frac{i}{\hbar} q \cdot \hat{p}}. \end{aligned}$$

□

Let's determine the action of a translation operator on a general state:

Proposition 2.4.4. *Consider a state $u \in L^2(\mathbb{R}^n)$. Then the action of the translation operator $\hat{T}_\Omega(x)$ on this state is the following:*

$$\left(\hat{T}_\Omega(x') u \right) (q) = e^{\frac{i}{\hbar} (q - \frac{1}{2} q') \cdot p'} u(q - q'). \quad (2.4.30)$$

Proof. By applying the previous corollary we have immediately that

$$\begin{aligned} \hat{T}_\Omega(x') u(q) &= e^{-\frac{i}{2\hbar} q' \cdot p'} e^{\frac{i}{\hbar} p' \cdot \hat{q}} e^{-\frac{i}{\hbar} q' \cdot \hat{p}} u(q) \\ &= e^{-\frac{i}{2\hbar} q' \cdot p'} e^{\frac{i}{\hbar} p' \cdot q} u(q - q') = e^{\frac{i}{\hbar} (q - \frac{1}{2} q') \cdot p'} u(q - q'). \end{aligned} \quad (2.4.31)$$

where we have used the fact that

$$e^{-\frac{i}{\hbar} q' \cdot \hat{p}} u(q) = u(q - q'). \quad (2.4.32)$$

□

On the Fourier side, we have the following similar result

$$\mathcal{F} \left(\hat{T}_\Omega(x')u \right) (p) = e^{-\frac{i}{\hbar}(p - \frac{1}{2}q') \cdot p'} (\mathcal{F}u) (p - p'). \quad (2.4.33)$$

The application of the translation operator can thus be interpreted as a translation of the state by $x = (q, p)$ in phase space.

2.5 Semiclassics

In this section we will review the background theory on the Wigner-Weyl transform which is the invertible mapping between the standard operator formulation of quantum mechanics in the Schrödinger picture and the phase-space formulation. In particular, we will introduce the mapping itself and two important objects, namely the Wigner function and the characteristic function which will be essential in what follows.

For what follows we will follow the framework and general notation of chapters 3 and 4 in Zworski's Semiclassical Analysis textbook [51] which is a comprehensive reference for all things semiclassical. We will leave a lot of proofs out here since this is meant to be a brief overview.

We start with the Fourier transform. In particular, we want to define a semiclassical Fourier transform which we will later use explicitly when considering the characteristic function. It will also provide insight into quantization.

Eventually we will want to allow our wavefunctions to be quite general in all that follows, but to build up to that point we need to introduce the Schwartz space, which will serve as a base space we will then build upon.

2.5.1 Schwartz space and the Fourier transform

In this section we use the following notation which is used throughout Zworski:

Definition 2.5.1.

$$D^\alpha = \frac{1}{i^{|\alpha|}} \partial^\alpha \quad (2.5.1)$$

where α is a multi-index, and hence $D_q^\alpha = \frac{1}{i^{|\alpha|}} \partial_q^\alpha$ and so on.

Definition 2.5.2 (Schwartz space). Define the *Schwartz space* as

$$\mathcal{S} = \mathcal{S}(\mathbb{R}^n) := \left\{ \phi \in C^\infty(\mathbb{R}^n) : \sup_{\mathbb{R}^n} |q^\alpha \partial^\beta \phi(q)| < \infty \quad \forall \text{ multiindices } \alpha, \beta \right\}. \quad (2.5.2)$$

This space has an associated family of seminorms

$$|\phi|_{\alpha, \beta} := \sup_{\mathbb{R}^n} |q^\alpha \partial^\beta \phi| \quad (2.5.3)$$

for each pair α, β and convergence of sequences is defined as

$$\phi_j \rightarrow \phi \text{ in } \mathcal{S} \quad (2.5.4)$$

if

$$|\phi_j - \phi|_{\alpha, \beta} \rightarrow 0 \quad \forall \alpha, \beta. \quad (2.5.5)$$

Basically, a function living in Schwartz space is a smooth function whose decay, and the decay of its derivatives, is faster than $|q|^{-m}$ for all possible m in \mathbb{N} .

We will also need to define the dual of \mathcal{S} , \mathcal{S}' which is the space of *tempered distributions*.

Definition 2.5.3 (Space of tempered distributions). We call \mathcal{S}' the space of tempered distributions and say that $u \in \mathcal{S}'$ if $u : \mathcal{S} \rightarrow \mathbb{C}$ is linear and $\phi_j \rightarrow \phi$ in \mathcal{S} implies $u(\phi_j) \rightarrow u(\phi)$.

Convergence in this space is defined as

$$u_j \rightarrow u \text{ in } \mathcal{S}' \quad (2.5.6)$$

if

$$u_j(\phi) \rightarrow u(\phi) \quad \forall \phi \in \mathcal{S}. \quad (2.5.7)$$

This space allows us to consider non-smooth expressions (for instance the dirac measure) and we will use it more explicitly when considering quantizations later as a way of extending our scope to more general functions.

Now we define the semiclassical Fourier transform.

Definition 2.5.4 (The scaled Fourier transform). Let $\hbar > 0$ be a small parameter, then the scaled Fourier transform is defined by

$$\mathcal{F}_\hbar \phi(p) := \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} \langle q, p \rangle} \phi(q) dq, \quad \phi \in \mathcal{S}. \quad (2.5.8)$$

As with the normal Fourier transform this has a well defined inverse

$$\mathcal{F}_\hbar^{-1} \psi(q) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar} \langle q, p \rangle} \psi(p) dp. \quad (2.5.9)$$

Note that this is often called the *semiclassical* Fourier transform in the maths literature. The usual properties of the Fourier transform also apply, we summarise these below:

Theorem 2.5.5 (Properties of the scaled Fourier Transform). *We have, for α a multi-index:*

$$(i) \quad (\hbar D_p)^\alpha \mathcal{F}_\hbar \phi = \mathcal{F}_\hbar((-q)^\alpha \phi), \quad (2.5.10)$$

$$(ii) \quad \mathcal{F}_\hbar((\hbar D_q)^\alpha \phi) = p^\alpha \mathcal{F}_\hbar \phi, \quad (2.5.11)$$

(iii)

$$\|\phi\|_{L^2} = \frac{1}{(2\pi\hbar)^{n/2}} \|\mathcal{F}_\hbar \phi\|_{L^2}. \quad (2.5.12)$$

The first two properties look somewhat complicated due to the presence of the multi-index, but for most important cases these just reduce down to the standard Fourier transform result that derivatives can be transformed into multiplication that we are used to. The only 'unusual' part is the parameter \hbar appearing to rescale everything. The last result is just a rescaling of the norm-preservation property.

2.5.2 Quantization formulas

We now introduce the concept of quantization so that we can begin to talk about our eventual target of the Wigner function.

Take the following function:

$$a = a(q, p) \in \mathcal{S}(\mathbb{R}^{2n}). \quad (2.5.13)$$

We will call a a *symbol*. We want to associate to this symbol an operator acting on functions $u = u(q)$. Think of how Hamiltonians in quantum mechanics are often expressed as a function of the position operator \hat{q} and the momentum operator $\hat{p} = \frac{\hbar}{i} \partial_q$. The idea of quantization is to generalise this relationship. There are a few common ways to do this which can be summarised in the following formula:

Definition 2.5.6 (Quantization operators). Define, for $a \in \mathcal{S}(\mathbb{R}^{2n})$, $u \in \mathcal{S}(\mathbb{R}^n)$ and $0 \leq t \leq 1$

$$\text{Op}_t(a)u(q) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar} \langle q-y, p \rangle} a(tq + (1-t)y, p) u(y) dy dp. \quad (2.5.14)$$

This is a *pseudo-differential operator*. In particular, define the choices

$$\text{Op}_{\frac{1}{2}}(a)u(q) = a^w(q, \hbar D_q) \quad (2.5.15)$$

and

$$\text{Op}_1(a)u(q) = a(q, \hbar D_q) \quad (2.5.16)$$

as the *Weyl* and *standard* quantizations respectively.

The difference here ultimately arises from the need to determine how one associates products of symbols to products of operators. For instance, for the product qp do we take $\hat{q}\hat{p}$ or $\hat{p}\hat{q}$ or perhaps $\frac{1}{2}(\hat{q}\hat{p} + \hat{p}\hat{q})$? The first of these, corresponds to the standard quantization, the second to the so-called anti-standard quantization, and the last, which places both \hat{p} and \hat{q} on an equal footing, corresponds to the Weyl quantization.

The Weyl quantization is the quantization that will primarily interest us. We can think of the symbols as our *classical observables* and the corresponding operators found via the above definition as the *quantum observables*.

As a remark, note that we can rescale to the case $\hbar = 1$ via the following change of variables:

$$\tilde{q} := \hbar^{-1/2}q, \quad \tilde{y} := \hbar^{-1/2}y, \quad \tilde{p} := \hbar^{-1/2}p. \quad (2.5.17)$$

In this case then we have that

$$a^w(q, \frac{\hbar}{i}\partial_q)u(q) = a_h^w(\tilde{q}, \frac{1}{i}\partial_q)\tilde{u}(\tilde{q}) \quad (2.5.18)$$

for

$$\tilde{u}(\tilde{q}) := u(q) = u(\hbar^{1/2}\tilde{q}), \quad a_h(\tilde{q}, \tilde{p}) := a(q, p) = a(\hbar^{1/2}\tilde{q}, \hbar^{1/2}\tilde{p}). \quad (2.5.19)$$

Remark 2.5.7. It is worth noting now the relationship between the standard quantization and the semiclassical Fourier transform. In particular, note that

$$a(q, \hbar D)u = \mathcal{F}_\hbar^{-1}(a(q, \cdot)\mathcal{F}_\hbar u(\cdot)). \quad (2.5.20)$$

This relationship does not hold for the Weyl quantization and as a result this makes many calculations easier with the standard quantization. However the standard quantization lacks many of the properties which make the Weyl quantization useful in practice.

The Weyl quantization does have the following simple form (see [51] Lemma 4.10) which relates it to the translation operators we introduced earlier:

Lemma 2.5.8 (Fourier Decomposition of a^w). *Define the Fourier transform of a symbol $a \in \mathcal{S}$ at the point $x' = (q', p') \in \mathbb{R}^{2n}$ to be*

$$\tilde{a}(x') = \int_{\mathbb{R}^{2n}} e^{-\frac{i}{\hbar}\langle x', x \rangle} a(x) dx. \quad (2.5.21)$$

Then the Fourier decomposition of the Weyl operator associated to a is given by

$$a^w(q, \hbar D_q) = \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} \tilde{a}(x') e^{\frac{i}{\hbar}(\langle q', q \rangle + \langle p', \hbar D_q \rangle)} dx' \quad (2.5.22)$$

or in terms of the translation operators we defined previously

$$a^w(q, \hbar D_q) = \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} \tilde{a}(x') \hat{T}(-x') dx'. \quad (2.5.23)$$

If we take $a \in \mathcal{S}'$, then this Fourier composition result also holds true if interpreted in the sense of tempered distributions.

We now extend our definition to more general distributional symbols in \mathcal{S}' .

Theorem 2.5.9 (Distributional symbols). *If $a \in \mathcal{S}'$, then $Op_t(a)$ can be defined as an operator mapping \mathcal{S} to \mathcal{S}' and for $0 \leq t \leq 1$*

$$Op_t(a) : \mathcal{S} \rightarrow \mathcal{S}' \quad (2.5.24)$$

is continuous.

Example 2.5.10. We will briefly give a few immediate examples that follow easily from the definitions above:

- (i) Let our symbol $a(q, p) = p^\alpha$, then for all $0 \leq t \leq 1$ we have

$$\text{Op}_t(a)u = (\hbar D_q)^\alpha u. \quad (2.5.25)$$

- (ii) If we take a polynomial symbol $a(q, p) = \sum_{|\alpha| \leq N} a_\alpha(q) p^\alpha$ then its standard quantization is simply

$$a(q, \hbar D_q) = \sum_{|\alpha| \leq N} a_\alpha(q) (\hbar D_q)^\alpha u. \quad (2.5.26)$$

- (iii) If we take our symbol to be the inner product $a(q, p) = \langle q, p \rangle$ then for all $0 \leq t \leq 1$

$$\text{Op}_t(a)u = (1 - t)\langle \hbar D_q, qu \rangle + t\langle q, \hbar D_q u \rangle \quad (2.5.27)$$

and in particular, the Weyl quantization is symmetrically given by

$$\langle q, \hbar D_q \rangle^w u = \frac{\hbar}{2} (\langle D_q, qu \rangle + \langle q, D_q u \rangle). \quad (2.5.28)$$

We now recall an important theorem (Theorem 4.1 in Zworski [51] quoted almost verbatim):

Theorem 2.5.11 (Schwartz class symbols). *Let us assume we have a symbol $a \in \mathcal{S}$. Then we have the following important results:*

- (i) *For each $0 \leq t \leq 1$, $\text{Op}_t(a)$ can be defined as an operator mapping \mathcal{S} to \mathcal{S} ; and furthermore*

$$\text{Op}_t(a) : \mathcal{S}' \rightarrow \mathcal{S}' \quad (2.5.29)$$

is continuous.

- (ii) *The formal adjoint is given by*

$$\text{Op}_t(a)^* = \text{Op}_{1-t}(\bar{a}) \quad (2.5.30)$$

- (iii) *In particular, the Weyl quantization of a real symbol is self-adjoint:*

$$a^w(q, \hbar D_q)^* = a^w(q, \hbar D_q) \text{ if } a \text{ is real.} \quad (2.5.31)$$

Now for the other direction (theorem 4.2 in Zworski).

Theorem 2.5.12. *If we take $a \in \mathcal{S}'$ then $\text{Op}_t(a)$ can be defined as an operator mapping \mathcal{S} to \mathcal{S}' and further than this*

$$\text{Op}_t(a) : \mathcal{S} \rightarrow \mathcal{S}' \quad (2.5.32)$$

for $0 \leq t \leq 1$ is continuous.

Now let's introduce the following result for the trace.

Lemma 2.5.13. *For $\hat{A} = A^w$, $\hat{B} = B^w$ Weyl quantizations of symbols $A(x)$ and $B(x)$ respectively, we have that*

$$\mathrm{tr}(\hat{A}\hat{B}) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} A(x)B(x)dx. \quad (2.5.33)$$

Proof. We use from (2.2.18) that

$$\mathrm{tr}(\hat{A}) = \int_{\mathbb{R}^n} K_A(q, q) dq \quad (2.5.34)$$

and by resolution of identity we have that

$$\mathrm{tr}(\hat{A}\hat{B}) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} K_A(q, q') K_B(q', q) dq dq'. \quad (2.5.35)$$

Using the quantization definition (2.5.14) we have

$$\mathrm{tr}(\hat{A}\hat{B}) = \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(q-q') \cdot (p-p')} A\left(\frac{q+q'}{2}, p\right) B\left(\frac{q+q'}{2}, p'\right) dp dp' dq dq' \quad (2.5.36)$$

and making the substitution $u = \frac{q+q'}{2}$ and $v = q - q'$ we have

$$\begin{aligned} \mathrm{tr}(\hat{A}\hat{B}) &= \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}v \cdot (p-p')} A(u, p) B(u, p') du dv dp dp' \\ &= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \delta(p - p') A(u, p) B(u, p') du dp dp' \\ &= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} A(u, p) B(u, p) du dp \\ &= \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} A(x) B(x) dx. \end{aligned} \quad (2.5.37)$$

where we have performed the v integral and then used the resulting delta function to eliminate p' . \square

We now note the following result which gives us a necessary and sufficient condition for Op_t to be Hilbert-Schmidt :

Corollary 2.5.14 (Hilbert-Schmidt quantizations). *Let $a \in \mathcal{S}'(\mathbb{R}^{2n})$. Then $\mathrm{Op}_t(a)$ is a Hilbert-Schmidt operator if and only if $a \in L^2(\mathbb{R}^{2n})$. In this case, we have that the Hilbert-Schmidt norm is given by:*

$$\|a^w\|_{HS}^2 = \frac{1}{(2\pi\hbar)^n} \int \int |a(q, p)|^2 dq dp. \quad (2.5.38)$$

Proof. If we take $\hat{A} = a^w$ and $\hat{B} = (a^w)^*$ in Lemma 2.5.13, then immediately we have that, using as well the result (2.2.19), that

$$\|a^w\|_{HS}^2 = \text{tr}(a^w(a^w)^*) = \frac{1}{(2\pi\hbar)^n} \int \int |a(q, p)|^2 dq dp, \quad (2.5.39)$$

giving the result. \square

Note that this result actually holds for any quantization. We would like to determine a similar result for operators in trace class, but this is not so straightforward and a complete characterization cannot be given. Instead we will only present a sufficient condition for an operator to be of trace class. Proving these results can be quite involved and for brevity we will simply state them in the form we need. The full results as well as the proofs behind them are given in chapter 9 of [7].

Theorem 2.5.15 (Trace class quantizations [7]). *Let $a \in \mathcal{S}'(\mathbb{R}^{2n})$ satisfy*

$$\sum_{|\alpha| \leq 2n+1} \hbar^{\frac{|\alpha|}{2}} \|\partial_{q,\theta}^\alpha a\|_{L^1} < \infty. \quad (2.5.40)$$

Then $Op_{\frac{1}{2}}(a) = a^w$ is of trace class and

$$\text{tr } a^w = \frac{1}{(2\pi\hbar)^n} \int \int a(q, p) dq dp \quad (2.5.41)$$

or more generally

$$\text{tr } Op_t(a) = \frac{1}{(2\pi\hbar)^n} \int \int a(q, p) dq dp \quad (2.5.42)$$

for all $t \in [0, 1]$.

2.5.3 Composition and an inverse

In this section we will briefly cover the fundamental composition result for the Weyl quantization, as well as some useful semiclassical expansions that can be used to simplify things in some cases. We will also cover an *inverse* of the Weyl quantization. With these two results we will have all the tools we need to derive the phase space Lindblad equation.

We'll start by introducing a composition result. Suppose we have two operators a^w and b^w which are associated to symbols a and b respectively. We wish to find the symbol c that under Weyl quantization gives us the product of the two operators a^w and b^w . That is, we want to find a symbol c such that

$$c^w = a^w b^w.$$

Following theorem 4.11 in Zworski [51] we have

Theorem 2.5.16 (Composition for the Weyl quantization). *Suppose $a, b \in \mathcal{S}$. Then we have*

$$a^w(q, \hbar D_q) b^w(q, \hbar D_q) = (a \star b)^w(q, \hbar D_q) \quad (2.5.43)$$

where the symbol $a \star b$ is defined by

$$a \star b(q, p) = e^{\frac{i\hbar}{2}\omega(\partial_q, \partial_p, \partial_y, \partial_\eta)} (a(q, p)b(y, \eta)) \Big|_{y=q, \eta=p}. \quad (2.5.44)$$

Here ω is the standard symplectic inner product. That is

$$\omega(\partial_q, \partial_p, \partial_y, \partial_\eta) = \partial_q \partial_\eta - \partial_p \partial_y. \quad (2.5.45)$$

We also have the integral representation of the symbol $a \star b$ given by

$$a \star b(q, p) = \frac{1}{(\pi \hbar)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{2i}{\hbar}\omega(w_1, w_2)} a(x + w_1) b(x + w_2) dw_1 dw_2. \quad (2.5.46)$$

for $x = (q, p)$.

Often in practice it is easier to work with the following:

Remark 2.5.17. We can also write the composition result as

$$f(q, p) \star g(q, p) = f(q, p) e^{\frac{i\hbar}{2} \overleftarrow{\nabla} \cdot \Omega \overrightarrow{\nabla}} g(q, p) \quad (2.5.47)$$

where

$$\Omega = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix} \quad (2.5.48)$$

is the standard symplectic matrix as defined in (2.3.9).

Here we have that $\nabla = \begin{pmatrix} \partial_q \\ \partial_p \end{pmatrix}$ and the notation $\overleftarrow{\nabla}$ is used to mean that the derivatives apply only to the left or equivalently for $\overrightarrow{\nabla}$ to the right. We now introduce some useful semiclassical expansions of this product which allow us to better understand it.

Theorem 2.5.18. *Let $N \in \mathbb{N}_0$. Then by expanding the exponential in (2.5.44) we have*

$$(a \star b)(q, p) = \sum_{k=0}^N \frac{i^k \hbar^k}{2^k k!} \omega(\partial_q, \partial_p, \partial_y, \partial_\eta)^k (a(q, p)b(y, \eta)) \Big|_{y=q, \eta=p} + O_{\mathcal{S}}(\hbar^{N+1}) \quad (2.5.49)$$

as $\hbar \rightarrow 0$. Expanding semiclassically explicitly in the lowest orders we have

$$a \star b = ab + \frac{i\hbar}{2} \{a, b\} + O_{\mathcal{S}}(\hbar^2) \quad (2.5.50)$$

which means that the commutator of the operators a^w and b^w is given simply by the Poisson bracket:

$$[a^w(q, \hbar D_q), b^w(q, \hbar D_q)] = i\hbar \{a, b\}^w(q, \hbar D_q) + O_{\mathcal{S}}(\hbar^3). \quad (2.5.51)$$

Note that when we say a function is $O_{\mathcal{S}}(\hbar^k)$ we mean that

$$|\phi|_{\alpha,\beta} := \sup_{\mathbb{R}^n} |q^\alpha \partial^\beta \phi| \leq C_{\alpha,\beta} \hbar^k \quad (2.5.52)$$

as $\hbar \rightarrow 0$ for all multiindices α, β .

This relation between the commutator of the operators a^w and b^w and the Poisson bracket of their associated symbols on phase space is a key example of the underlying correspondence principle between classical and quantum mechanics.

Finally, let us introduce the inverse of Weyl quantization, often known as the *Wigner map*. This allows us to determine a symbol associated to a given operator and will be important when transforming our Lindblad equation to a phase space equivalent.

To construct this inverse, let's begin with the integral form of our Weyl quantization and apply it to a wavefunction $\psi(q)$:

$$a^w \psi(q) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(q-y) \cdot p} a\left(\frac{q+y}{2}, p\right) \psi(y) dy dp = \int_{\mathbb{R}^n} K(q, y) \psi(y) dy \quad (2.5.53)$$

where $K(q, y)$ is the Schwartz kernel defined by

$$K(q, y) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}(q-y) \cdot p} a\left(\frac{q+y}{2}, p\right) dp. \quad (2.5.54)$$

Now if we make the transformation $q \rightarrow q + \frac{y}{2}$ and $y \rightarrow q - \frac{y}{2}$ we get

$$K\left(q + \frac{y}{2}, q - \frac{y}{2}\right) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^n} e^{\frac{i}{\hbar}y \cdot p} a(q, p) dp \quad (2.5.55)$$

Note then that this is a Fourier inverse formula and hence if we take the Fourier transform w.r.t y we get that

$$\int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}y \cdot \eta} K\left(q + \frac{y}{2}, q - \frac{y}{2}\right) dy = a(q, \eta) \quad (2.5.56)$$

Hence, if we know the kernel of our operator $K(q, y)$ then we can determine the symbol associated to our operator using the above result. As we saw in (2.1.9), for a general operator \hat{A} , the kernel in the position representation can be defined by

$$K_{\hat{A}}(q, y) = \langle q | \hat{A} | y \rangle. \quad (2.5.57)$$

A particularly important case for our purposes is the case where the operator we wish to find the symbol of is the *density operator* of our system. If we denote this by $\hat{\rho}$ then we can define the following

Definition 2.5.19 (The Wigner function). Consider a density operator $\hat{\rho}$. Then the symbol associated to this operator which we denote by ρ is given by

$$\rho(x) = \rho(q, p) = \int_{\mathbb{R}^n} \left\langle q + \frac{y}{2} \middle| \hat{\rho} \middle| q - \frac{y}{2} \right\rangle e^{-\frac{i}{\hbar}p \cdot y} dy. \quad (2.5.58)$$

Then we define the Wigner function for this operator to be

$$W(x) = W(q, p) = \frac{1}{(2\pi\hbar)^n} \rho(q, p). \quad (2.5.59)$$

Note that we will often refer to the symbol of the operator $\hat{\rho}$ as the “Wigner function” since it differs merely by a factor $\frac{1}{(2\pi\hbar)^n}$. This factor is there because it is needed to normalise traces, but including it can make things more complicated in some situations.

Finally for this section we introduce the *characteristic function* of an operator.

Definition 2.5.20 (The characteristic function). The characteristic function $\chi_\rho(\xi)$ is the Fourier transform of the Wigner function of $\hat{\rho}$

$$\chi_\rho(\xi) := \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} e^{-\frac{i}{\hbar}\xi \cdot x} \rho(t, x) dx = \text{tr} \left[\hat{T}(\xi) \hat{\rho} \right] \quad (2.5.60)$$

where $\hat{T}(\xi)$ is the standard Weyl-Heisenberg translation operator defined previously. Note that this is not the *twisted* operator.

The fact that we can write the characteristic in either of these forms is a consequence of lemma (2.5.13), taking $\hat{A} = \hat{T}(\xi)$ and $\hat{B} = \hat{\rho}$.

2.5.4 Symbol classes

In this section we present some sufficient conditions for quantized operators to be bounded and trace class by introducing the concept of symbol classes. Here we will again follow Zworski [51] quite closely.

Firstly, we define the concept of an order function.

Definition 2.5.21 (Order function). We define a measurable function $m : \mathbb{R}^{2n} \rightarrow (0, \infty)$ as an order function if there exists constants C, N such that

$$m(w) \leq C \langle x - w \rangle^N m(x) \quad \forall w, x \in \mathbb{R}^{2n}. \quad (2.5.61)$$

Note here that the object $\langle x \rangle$ is defined as

$$\langle x \rangle = (1 + |x|^2)^{\frac{1}{2}} \quad (2.5.62)$$

and is known as a *Japanese bracket* in PDE theory.

Some standard choices of order functions are

$$m(x) \equiv 1, \quad (2.5.63)$$

$$m(x) = \langle q \rangle^a \langle p \rangle^b, \quad (2.5.64)$$

for $a, b \in \mathbb{R}$ and

$$m(x) = \langle x \rangle^a \quad (2.5.65)$$

for $a \in \mathbb{R}$. Note here that if we have two order functions m_1, m_2 then the product $m_1 m_2$ is also an order functions.

Having defined order functions we can now define the concept of a symbol class.

Definition 2.5.22 (Symbol classes). Suppose we have an order function m on \mathbb{R}^{2n} , then define the class of symbols $S(m)$ as

$$S(m) := \{a \in C^\infty \mid \forall \alpha \exists C_\alpha \text{ s.t. } |\partial^\alpha a| \leq C_\alpha m\}. \quad (2.5.66)$$

where α are multiindices and C_α are constants. Now let's extend this to a \hbar dependent definition for $\delta \geq 0$ as follows:

$$S_\delta(m) := \left\{a \in C^\infty \mid |\partial^\alpha a| \leq C_\alpha \hbar^{-\delta|\alpha|} m \quad \forall \alpha\right\} \quad (2.5.67)$$

Note that symbols in both classes (not just S_δ) can depend on \hbar . If this is the case, then the constants C_α must be uniform for $0 < \hbar \leq \hbar_0$ for some $\hbar_0 > 0$.

As a remark, note that, for $a \in S_\delta$ then

$$|\partial^\alpha a_\hbar| = \hbar^{\frac{|\alpha|}{2}} |\partial^\alpha a| \leq C_\alpha \hbar^{|\alpha|(\frac{1}{2}-\delta)} \quad (2.5.68)$$

for each multiindex α . Here a_\hbar is the standard rescaling described previously in (2.5.19). The right hand side is clearly unbounded for $\delta > \frac{1}{2}$. The value $\delta = \frac{1}{2}$ is critical, that is we do not get any decay as $\hbar \rightarrow 0$ for $|\alpha| > 0$. As a result, it is common to take the choice $\delta \in [0, 1/2]$.

Finally, we note that for our purposes in this thesis we will in general not need complicated order functions $m(x)$. Primarily, we will use order functions of the form

$$m(x) = \langle x \rangle^m \quad (2.5.69)$$

where $m \in \mathbb{R}$ and in this case we will simply denote the symbol classes by the shorthand

$$S_\delta^m := \left\{a \in C^\infty \mid |\partial^\alpha a| \leq C_\alpha \hbar^{-\delta|\alpha|} \langle x \rangle^m \quad \forall \alpha\right\}. \quad (2.5.70)$$

Having introduced symbol classes, we can now state the following very important results (Theorem 4.16 and 4.23 in Zworski [51] quoted verbatim):

Theorem 2.5.23 (Quantizing general symbols). *If $a \in S_\delta(m)$, then*

$$a^w(q, \frac{\hbar}{i}\partial_q) : \mathcal{S} \rightarrow \mathcal{S} \quad (2.5.71)$$

and

$$a^w(q, \frac{\hbar}{i}\partial_q) : \mathcal{S}' \rightarrow \mathcal{S}' \quad (2.5.72)$$

are continuous linear transformations.

Let's now consider the symbol class associated to the star product of two symbols a and b :

Theorem 2.5.24 (The symbol class of $a \star b$). *Let $a \in S_\delta(m_1)$ and $b \in S_\delta(m_2)$, then we have*

(i)

$$a \star b \in S_\delta(m_1 m_2), \quad (2.5.73)$$

and we have

$$a^w(q, \hbar D) b^w(q, \hbar D) = (a \star b)^w(q, \hbar D) \quad (2.5.74)$$

as equivalent operators from $\mathcal{S} \rightarrow \mathcal{S}$.

(ii) Further to this, we have the expansion

$$a \star b = ab + \frac{i}{2\hbar} \{a, b\} + O_{S_\delta(m_1 m_2)}(\hbar^{1-2\delta}) \quad (2.5.75)$$

and the commutator

$$[a^w(q, \hbar D), b^w(q, \hbar D)] = \frac{\hbar}{i} \{a, b\}^w(q, \hbar D) + O_{S_\delta(m_1 m_2)}(\hbar^{3(1-2\delta)}). \quad (2.5.76)$$

We now have the following theorem on the L^2 boundedness of quantized symbols

Theorem 2.5.25 (L^2 boundedness for symbols in S). (i) For a symbol $a \in S(m)$, the Weyl quantization

$$a^w(q, D) : L^2(\mathbb{R}^2) \rightarrow L^2(\mathbb{R}^n) \quad (2.5.77)$$

is a bounded operator, with the estimate

$$\|a^w(q, D)\|_{L^2 \rightarrow L^2} \leq C \sum_{\alpha \leq 2n+1} \sup_{\mathbb{R}^n} |\partial^\alpha a|. \quad (2.5.78)$$

(ii) If $a \in S_\delta(m)$ where $\delta \in [0, 1/2]$, then

$$\|a^w(q, \hbar D)\|_{L^2 \rightarrow L^2} \leq C \sum_{\alpha \leq 2n+1} \hbar^{\frac{|\alpha|}{2}} \sup_{\mathbb{R}^n} |\partial^\alpha a|. \quad (2.5.79)$$

Finally, we note the following result about composition of operators in S_δ :

Corollary 2.5.26 (Composition and multiplication). Let $a, b \in S_\delta$ for $0 \leq \delta < \frac{1}{2}$. Then

$$(ab)^w(q, \frac{1}{i} \partial_q) = a^w(q, \frac{1}{i} \partial_q) b^w(q, \frac{1}{i} \partial_q) + O_{L^2 \rightarrow L^2}(\hbar^{1-2\delta}). \quad (2.5.80)$$

Hence if we choose a and b to be in appropriate symbol classes, then the operator associated with their product will be L^2 bounded as well.

Finally we note that similar results hold for guaranteeing a quantized symbol is trace class. By comparing the definition of the symbol class $S_\delta(m)$ with the trace class condition (2.5.40) we see that for $a \in S_\delta(m)$, $0 \leq \delta \leq 1/2$, that a^w is of trace class.

2.6 The Lindblad equation on phase space

In this section we will use the results described above where we introduced semiclassical theory to translate our operator form of the Lindblad equation (2.2.54) to an equation on phase space.

Recall that we had the following form of the Lindblad equation (2.2.54):

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \frac{1}{2\hbar} \sum_j [\hat{L}_j \hat{\rho}, \hat{L}_j^\dagger] - [\hat{\rho} \hat{L}_j^\dagger, \hat{L}_j]. \quad (2.6.1)$$

where $\hat{\rho}$ is our density operator, \hat{H} is our internal Hamiltonian operator, and the operators \hat{L}_k are our Lindblad terms which describe interaction with the environment.

Assume now that each of these operators are the Weyl quantization (see (2.5.15)) of an associated phase space symbol ρ, H, L_k respectively. For our purposes we will consider initial ρ_0 's in the form of a Gaussian, which is hence in $S_{\frac{1}{2}}^{-\infty}$ and $H \in S_0^2$ and $L \in S_0^1$. Recall that the Weyl quantization is independent of time and that we had from Theorem (2.5.16) the following composition result

$$a^w b^w = (a \star b)^w \quad (2.6.2)$$

where \star denotes the star product. Using this, we can rewrite the Lindblad equation as

$$\begin{aligned} \left(\frac{\partial \rho}{\partial t} \right)^w &= -\frac{i}{\hbar} (H \star \rho)^w + \frac{i}{\hbar} (\rho \star H)^w \\ &\quad + \frac{1}{\hbar} \sum_j (L_j \star \rho \star \bar{L}_j)^w - \left(\frac{1}{2} \bar{L}_j \star L_j \star \rho \right)^w - \left(\frac{1}{2} \rho \star \bar{L}_j \star L_j \right)^w \end{aligned} \quad (2.6.3)$$

which after rearranging using the fact that the Weyl quantization is linear, and dropping the quantization notation gives us the following equation for the evolution of the symbols associated to the operators of our equation on phase space:

$$i\hbar \frac{\partial \rho}{\partial t} = H \star \rho - \rho \star H + i \sum_j L_j \star \rho \star \bar{L}_j - \frac{1}{2} \bar{L}_j \star L_j \star \rho - \frac{1}{2} \rho \star \bar{L}_j \star L_j. \quad (2.6.4)$$

This equation is the fundamental equation we will be studying in this thesis. Recall that the symbol product admitted a semiclassical expansion (2.5.50)

$$a \star b = ab + \frac{i\hbar}{2} \{a, b\} + O(\hbar^2). \quad (2.6.5)$$

Hence, the commutator of two operators can be written in terms of their symbols as

$$[a^w, b^w] = \frac{\hbar}{i} \{a, b\}^w + O(\hbar^3). \quad (2.6.6)$$

Note that the error term being of order \hbar^3 is specific to the Weyl quantization. In the standard quantization for instance this would be of $O(\hbar^2)$.

In particular then, note that we can rewrite our Lindblad equation on phase space (2.6.4) as the following expansion:

Proposition 2.6.1. *The Lindblad equation (2.2.54) has an associated symbol equation on phase space with the following expansion to lowest orders in \hbar*

$$\begin{aligned} i\hbar \frac{\partial \rho}{\partial t} = i\hbar \{H, \rho\} - \frac{\hbar}{2} \sum_j \{L_j \rho, \bar{L}_j\} - \{\bar{L}_j \rho, L_j\} \\ - \frac{i\hbar^2}{4} \sum_j \{L_j, \{\rho, \bar{L}_j\}\} + \{\bar{L}_j, \{\rho, L_j\}\} + O(\hbar^3) \end{aligned} \quad (2.6.7)$$

where ρ, H and the L_j 's are the symbols associated to the operators $\hat{\rho}, \hat{H}$ and \hat{L}_j 's.

Proof. We start by noting that

$$H \star \rho - \rho \star H = i\hbar \{H, \rho\} + O(\hbar^3) \quad (2.6.8)$$

as this is simply the commutator result (2.6.6). Now we write the Lindblad terms as

$$\begin{aligned} [\hat{L}_j \hat{\rho}, \hat{L}_j^\dagger] - [\hat{\rho} \hat{L}_j^\dagger, \hat{L}_j] = \text{Op}_{\frac{1}{2}} [(L_j \star \rho) \star \bar{L}_j - \bar{L}_j \star (L_j \star \rho)] \\ - \text{Op}_{\frac{1}{2}} [(\rho \star \bar{L}_j) \star L_j - L_j \star (\rho \star \bar{L}_j)]. \end{aligned}$$

Dropping the $\text{Op}_{\frac{1}{2}}$ for notational convenience and expanding using (2.5.50) we have that

$$\begin{aligned} (L_j \star \rho) \star \bar{L}_j &= (L_j \star \rho) \bar{L}_j + \frac{i\hbar}{2} \{L_j \star \rho, \bar{L}_j\} + O(\hbar^3) \\ &= L_j \rho \bar{L}_j + \frac{i\hbar}{2} \{L_j, \rho\} \bar{L}_j \\ &\quad + \frac{i\hbar}{2} \left[\{L_j \rho, \bar{L}_j\} + \frac{i\hbar}{2} \{\{L_j, \rho\}, \bar{L}_j\} \right] + O(\hbar^3) \end{aligned}$$

Repeating this process for the term $\bar{L}_j \star (L_j \star \rho)$ we see that

$$\begin{aligned} \bar{L}_j \star (L_j \star \rho) &= \bar{L}_j L_j \rho + \frac{i\hbar}{2} \bar{L}_j \{L_j, \rho\} \\ &\quad + \frac{i\hbar}{2} \left[\{\bar{L}_j, L_j \rho\} + \frac{i\hbar}{2} \{\bar{L}_j, \{L_j, \rho\}\} \right] + O(\hbar^3). \end{aligned}$$

If we take the difference of these two terms we see that the first two parts cancel and we are left with

$$(L_j \star \rho) \star \bar{L}_j - \bar{L}_j \star (L_j \star \rho) = i\hbar \{L_j \rho, \bar{L}_j\} - \frac{\hbar^2}{2} \{\{L_j, \rho\}, \bar{L}_j\} + O(\hbar^3). \quad (2.6.9)$$

If we repeat this process for the second commutator, we have that

$$(\rho \star \bar{L}_j) \star L_j - L_j \star (\rho \star \bar{L}_j) = i\hbar \{\rho \bar{L}_j, L_j\} - \frac{\hbar^2}{2} \{\{\rho, \bar{L}_j\}, L_j\} + O(\hbar^3). \quad (2.6.10)$$

Combining these two results we arrive at the following form of the Lindblad equation on phase space

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} + \frac{1}{2\hbar} \sum_j i\hbar (\{L_j \rho, \bar{L}_j\} - \{\rho \bar{L}_j, L_j\}) \quad (2.6.11)$$

$$+ \frac{1}{2\hbar} \sum_j \left(-\frac{\hbar^2}{2} \right) (\{\{\rho, \bar{L}_j\}, L_j\} - \{\{\rho, \bar{L}_j\}, L_j\}) + O(\hbar^3). \quad (2.6.12)$$

If we now multiply through by $i\hbar$ and use the fact that the Poisson bracket is anti-symmetric, we arrive at the result (2.6.7). \square

2.6.1 Linear Lindblads and quadratic Hamiltonians

The terms of higher order in \hbar involve higher order derivatives of H and L_j and in particular, if we choose H at most quadratic in q and p and the L_j 's at most linear, then all these higher order terms are zero and the above form becomes exact.

This is particularly useful because in many cases these restrictions are satisfied. For instance, if we take an internal harmonic oscillator Hamiltonian and a heat bath model of the environment described by creation and annihilation operators as we saw for the example in 2.2.5. In that case we have the exact equation

$$\begin{aligned} i\hbar \frac{\partial \rho}{\partial t} = i\hbar \{H, \rho\} - \frac{\hbar}{2} \sum_j \{L_j \rho, \bar{L}_j\} - \{\bar{L}_j \rho, L_j\} \\ - \frac{i\hbar^2}{4} \sum_j \{L_j, \{\rho, \bar{L}_j\}\} + \{\bar{L}_j, \{\rho, L_j\}\}. \end{aligned} \quad (2.6.13)$$

It can be useful to rewrite this equation in the form

$$\partial_t \rho = X_0 \rho + \nabla \cdot X_0 \rho + \frac{\hbar}{2} \sum_{k=1}^{2K} X_k^2 \rho \quad (2.6.14)$$

where K is the total number of Lindblad operators and the vector fields X_0, X_1, \dots, X_{2K} are given as follows:

$$X_0 \rho = \{H, \rho\} + \sum_k \text{Im } L_k \{\text{Re } L_k, \rho\} - \text{Re } L_k \{\text{Im } L_k, \rho\}, \quad (2.6.15)$$

where by direct calculation we see that

$$\nabla \cdot X_0 = 2 \sum_k \{\text{Re } L_k, \text{Im } L_k\} \quad (2.6.16)$$

and

$$X_k \rho = \{\text{Re } L_k, \rho\}, \quad X_{K+k} \rho = \{\text{Im } L_k, \rho\} \quad (2.6.17)$$

for $k = 1, \dots, K$. This form of the Lindblad equation allows us to identify both the drift described by the vector field X_0 and the dispersive part of the equation described by the vector fields X_k^2 as well as the term $\nabla \cdot X_0$ preserving phase space volumes.

Since we are considering quadratic $H(x)$ and linear $L_k(x)$ we can make some simplifications. We introduce a parametrization that we will use extensively in this thesis. We write

$$L_k(x) = \omega(x, l_k) = x \cdot \Omega l_k, \quad (2.6.18)$$

where

$$l_k = \operatorname{Re} l_k + i \operatorname{Im} l_k \in \mathbb{C}^{2n}. \quad (2.6.19)$$

Then, with this notation,

$$X_k \rho = \{\operatorname{Re} L_k, \rho\} = \operatorname{Re} l_k \cdot \nabla \rho, \quad (2.6.20)$$

and

$$X_{K+k} \rho = \{\operatorname{Im} L_k, \rho\} = \operatorname{Im} l_k \cdot \nabla \rho. \quad (2.6.21)$$

Hence the vector fields are constant and given by $\operatorname{Re} l_k$ and $\operatorname{Im} l_k$. Also, for quadratic $H(x)$ we have the Hamiltonian map $F : \mathbb{R}^{2n} \rightarrow \mathbb{R}^{2n}$ defined by

$$\omega(Fx, x) = H(x) \implies F = \Omega H'' \quad (2.6.22)$$

where H'' is the $2n \times 2n$ Hessian of $H(x)$, which is constant. With this we have

$$\{H, \rho\}(x) = -(Fx) \cdot \nabla \rho(x). \quad (2.6.23)$$

Using these results, we can rewrite the vector fields as

$$X_0 \rho = (-Ax) \cdot \nabla \rho \quad \text{and} \quad \sum_{k=1}^{2K} X_k^2 \rho = \nabla \cdot M \nabla \rho, \quad (2.6.24)$$

where

$$A = F + N\Omega \quad (2.6.25)$$

with

$$N = \sum_k \operatorname{Re} l_k \operatorname{Im} l_k^T - \operatorname{Im} l_k \operatorname{Re} l_k^T, \quad M = \sum_k \operatorname{Re} l_k \operatorname{Re} l_k^T + \operatorname{Im} l_k \operatorname{Im} l_k^T. \quad (2.6.26)$$

Note that

$$\sum_k \bar{l}_k l_k^T = M + iN \quad (2.6.27)$$

and that M is symmetric and N is anti-symmetric.

We can use these results to write our phase space Lindblad equation as

$$\partial_t \rho = -(Ax) \cdot \nabla \rho - \operatorname{tr}(A) \rho + \frac{\hbar}{2} \nabla \cdot M \nabla \rho. \quad (2.6.28)$$

2.7 Gaussian states

2.7.1 General Gaussian states

We now introduce the concept of a Gaussian coherent state as these will be the main states of interest in this thesis. While on the surface this may seem like a big restriction, as we will see the Gaussian coherent states are an extremely useful tool for our investigations and, because the set of Gaussian coherent states forms an overcomplete basis, we can extend the results that we obtain to more general states easily.

These states can be traced back to the work of Schrödinger when looking for solutions of the Schrödinger equation that satisfied the correspondence principle. For the case of the quantum harmonic oscillator, he found what would later be called coherent states as the states whose dynamics resembled the dynamics of the classical operator most closely. These states are minimum uncertainty and their evolution is concentrated along the classical trajectories of the system.

If we assume our base state u_0 is in Schwartz space $\mathcal{S}(\mathbb{R}^n)$ then for a given x

$$u_x(q) = (\hat{T}_\Omega(x)u_0)(q) \quad (2.7.1)$$

is the associated coherent state, where $\hat{T}_\Omega(x)$ is the twisted Weyl-Heisenberg translation operator (2.4.6). A particularly useful subset that we will use throughout this thesis are the following Gaussian states:

Definition 2.7.1 (Gaussian coherent states). Let B be an $n \times n$ complex symmetric matrix such that $\text{Im } B$ is positive definite. Then we can define our base state u_0 to be the following Gaussian state:

$$\psi_0^B(q) = \frac{(\det \text{Im } B)^{1/4}}{(\pi \hbar)^{n/4}} e^{\frac{i}{2\hbar} q \cdot B q} \quad (2.7.2)$$

and by applying the translation operator $\hat{T}_\Omega(X)$ for $X = (Q, P)$ we arrive at the set of generalised Gaussian coherent states:

$$\psi_X^B(q) = \frac{(\det \text{Im } B)^{1/4}}{(\pi \hbar)^{n/4}} e^{-\frac{i}{2\hbar} Q \cdot P} e^{\frac{i}{\hbar} \left(\frac{1}{2}(q-Q) \cdot B(q-Q) + P \cdot (q-Q) \right)}. \quad (2.7.3)$$

Note that while in principle the phase factor $e^{-\frac{i}{2\hbar} Q \cdot P}$ should always be present, in practice for our purposes this prefactor can always be absorbed into constants. Hence, in some cases we may drop this and take

$$\psi_X^B(q) = \frac{(\det \text{Im } B)^{1/4}}{(\pi \hbar)^{n/4}} e^{\frac{i}{\hbar} \left(\frac{1}{2}(q-Q) \cdot B(q-Q) + P \cdot (q-Q) \right)}. \quad (2.7.4)$$

as our definition of a Gaussian coherent state.

2.7.2 The Wigner function of a Gaussian state

Having defined our general Gaussian state we now introduce its Wigner function which will be of great use to us. We have that, for $\psi_Z^B(q)$ as defined above, Wigner function of this state denoted by $W(q, p)$ is given by the following:

Proposition 2.7.2 (Wigner function of a Gaussian state). *For a state $\psi_X^B(q)$, the associated symbol on phase space is given by*

$$W(x) = \frac{1}{(\pi\hbar)^n} e^{\frac{i}{\hbar}(x-X) \cdot iG(x-X)} \quad (2.7.5)$$

where $x = (q, p)$, $X = (Q, P)$ and

$$G = \begin{pmatrix} \text{Im } B + \text{Re } B (\text{Im } B)^{-1} \text{Re } B & -\text{Re } B (\text{Im } B)^{-1} \\ -(\text{Im } B)^{-1} \text{Re } B & (\text{Im } B)^{-1} \end{pmatrix}. \quad (2.7.6)$$

Proof. Let $\psi_X^B(q)$ be our coherent state defined as above, and take as our density matrix the operator

$$\hat{\rho} := |\psi_X^B\rangle \langle \psi_X^B|. \quad (2.7.7)$$

The symbol associated to this operator is given by

$$\rho(q, p) = \int_{\mathbb{R}^n} \langle q + \frac{y}{2} | \hat{\rho} | q - \frac{y}{2} \rangle e^{-\frac{i}{\hbar} p \cdot y} dy. \quad (2.7.8)$$

Plugging in our $\hat{\rho}$ we have

$$\begin{aligned} \rho(q, p) &= \frac{(\det \text{Im } B)^{1/2}}{(\pi\hbar)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar} p \cdot y} e^{\frac{i}{\hbar} [\frac{1}{2}(q-Q+\frac{y}{2}) \cdot B(q-Q+\frac{y}{2}) + P \cdot (q-Q+\frac{y}{2})]} \\ &\quad \times e^{-\frac{i}{\hbar} [\frac{1}{2}(q-Q-\frac{y}{2}) \cdot B^*(q-Q-\frac{y}{2}) + P \cdot (q-Q-\frac{y}{2})]} dy \end{aligned} \quad (2.7.9)$$

Expanding and combining terms we arrive at the following:

$$\begin{aligned} \rho(q, p) &= \frac{(\det \text{Im } B)^{1/2}}{(\pi\hbar)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}(p-P) \cdot y} e^{\frac{i}{\hbar} [(q-Q) \cdot \frac{B-B^*}{2}(q-Q)]} \\ &\quad e^{\frac{i}{\hbar} [\frac{1}{2}(q-Q) \cdot \frac{B+B^*}{2}(p-P) + \frac{1}{2}(p-P) \cdot \frac{B+B^*}{2}(q-Q) + \frac{1}{4}(p-P) \cdot \frac{B-B^*}{2}(p-P)]} dy. \end{aligned} \quad (2.7.10)$$

Using that

$$\text{Re } B = \frac{B + B^*}{2}, \quad i \text{Im } B = \frac{B - B^*}{2} \quad (2.7.11)$$

we have (using that B is symmetric)

$$\begin{aligned} \rho(q, p) &= \frac{(\det \text{Im } B)^{1/2}}{(\pi\hbar)^{n/2}} e^{-\frac{1}{\hbar}(q-Q) \cdot \text{Im } B(q-Q)} \\ &\quad \int_{\mathbb{R}^n} e^{-\frac{i}{\hbar}(p-P) \cdot y} e^{-\frac{1}{4\hbar} y \cdot \text{Im } B y + \frac{i}{\hbar} \text{Re } B(q-Q) \cdot y} dy. \end{aligned} \quad (2.7.12)$$

Let $A = \frac{1}{2\hbar} \text{Im } B$ and $J = \frac{1}{\hbar} [\text{Re } B(q - Q) - (p - P)]$, then we can rewrite the integral as

$$I = \int_{\mathbb{R}^n} e^{-\frac{1}{2}y \cdot Ay + iJ \cdot y}. \quad (2.7.13)$$

This is now a simple Gaussian integral that has the standard result

$$I = \frac{(2\pi)^{n/2}}{(\det A)^{1/2}} e^{-\frac{1}{2}J \cdot A^{-1}J}. \quad (2.7.14)$$

Now simply plugging in our A and J we get

$$\det A = \frac{1}{(2\hbar)^n} \det \text{Im } B, \quad A^{-1} = 2\hbar(\text{Im } B)^{-1} \quad (2.7.15)$$

and hence

$$\begin{aligned} I = & \frac{2^n \pi^{n/2} \hbar^{n/2}}{(\det \text{Im } B)^{1/2}} \\ & \exp \left(-\frac{1}{\hbar} [(q - Q) \cdot \text{Re } B(\text{Im } B)^{-1} \text{Re } B(q - Q) - (q - Q) \cdot \text{Re } B(\text{Im } B)^{-1}(p - P) \right. \\ & \left. - (p - P) \cdot (\text{Im } B)^{-1} \text{Re } B(q - Q) + (p - P) \cdot (\text{Im } B)^{-1}(p - P)] \right). \end{aligned} \quad (2.7.16)$$

Using this we can write

$$\rho(q, p) = 2^n e^{-\frac{1}{\hbar}(x-X) \cdot G(x-X)} \quad (2.7.17)$$

where $x = (q, p)$, $X = (Q, P)$ as described before and

$$G = \begin{pmatrix} \text{Im } B + \text{Re } B(\text{Im } B)^{-1} \text{Re } B & -\text{Re } B(\text{Im } B)^{-1} \\ -(\text{Im } B)^{-1} \text{Re } B & (\text{Im } B)^{-1} \end{pmatrix}. \quad (2.7.18)$$

Using the fact that

$$W(q, p) = \frac{1}{(2\pi\hbar)^n} \rho(q, p) \quad (2.7.19)$$

we get the result. \square

2.7.3 The Wigner function of a superposition of Gaussian states

Often we wish to work with superpositions of Gaussian states $\psi_{X_j}^B$ which we write in terms of translation operators as

$$\psi = \frac{1}{\sqrt{\mathcal{N}}} \sum_{j=1}^N \hat{T}_\Omega(X_j) \psi_0 \quad (2.7.20)$$

where \mathcal{N} serves to normalise our state. Then the density operator is given directly by

$$\hat{\rho} = |\psi\rangle \langle\psi| = \frac{1}{\mathcal{N}} \sum_{j,k} \hat{T}_\Omega(X_j) |\psi_0\rangle \langle\psi_0| \hat{T}_\Omega^*(X_k) \quad (2.7.21)$$

and using the trace form of the characteristic function we find that

$$\chi_\rho(\xi) = \frac{1}{\mathcal{N}} \sum_{j,k} \text{tr} \left[\hat{T}_\Omega^*(X_k) \hat{T}(\xi) \hat{T}_\Omega(X_j) |\psi_0\rangle \langle\psi_0| \right]. \quad (2.7.22)$$

Using our composition relations for translation operators (2.4.17) we have that

$$\hat{T}_\Omega(X_k)^* \hat{T}(\xi) \hat{T}_\Omega(X_j) = e^{-\frac{i}{\hbar} \xi \cdot \bar{X}_{jk}} e^{\frac{i}{2\hbar} X_k \cdot \Omega X_j} \hat{T}_\Omega(\delta X_{jk} + \Omega \xi) \quad (2.7.23)$$

where $\bar{X}_{jk} = \frac{1}{2}(X_j + X_k)$ and $\delta X_{jk} = X_j - X_k$. Hence we see immediately that

$$\chi_\rho(\xi) = \frac{1}{\mathcal{N}} \sum_{j,k} e^{-\frac{i}{\hbar} \xi \cdot \bar{X}_{jk}} e^{\frac{i}{2\hbar} X_k \cdot \Omega X_j} \text{tr} \left[\hat{T}_\Omega(\delta X_{jk} + \Omega \xi) |\psi_0\rangle \langle\psi_0| \right]. \quad (2.7.24)$$

If we define the characteristic function of a single Gaussian state to be given by

$$\chi_g(\xi) = \text{tr} \left[\hat{T}(\xi) |\psi_0\rangle \langle\psi_0| \right] \quad (2.7.25)$$

where $g(x)$ is the Wigner function associated to a single coherent state centred at zero, then we get that

$$\chi_\rho(\xi) = \frac{1}{\mathcal{N}} \sum_{j,k} e^{-\frac{i}{\hbar} \xi \cdot \bar{X}_{jk}} e^{\frac{i}{2\hbar} X_k \cdot \Omega X_j} \chi_g(\xi - \Omega \delta X_{jk}) \quad (2.7.26)$$

or

$$\chi_\rho(\xi) = \frac{1}{\mathcal{N}} \sum_k e^{-\frac{i}{\hbar} \xi \cdot X_k} \chi_g(\xi) + \frac{1}{\mathcal{N}} \sum_{j \neq k} e^{\frac{i}{\hbar} \xi \cdot \bar{X}_{jk}} e^{\frac{i}{2\hbar} X_k \cdot \Omega X_j} \chi_g(\xi - \Omega \delta X_{jk}). \quad (2.7.27)$$

If we now take the inverse Fourier transform, then we arrive at the following result for the Wigner function of a superposition of coherent states:

$$\rho(x) = \frac{1}{\mathcal{N}} \sum_k g(x - X_k) + \frac{1}{\mathcal{N}} \sum_{j \neq k} e^{\frac{i}{2\hbar} X_k \cdot \Omega X_j} e^{-\frac{i}{\hbar} x \cdot \Omega^T \delta X_{kj}} g(x - \bar{X}_{kj}). \quad (2.7.28)$$

The first term corresponds to a probability distribution arising from the convex combination of the distributions of the individual states $\hat{T}_\Omega(X_j) \psi_0$, while the second sum represents the interference between the individual states in this superposition. For $\delta X_{jk} \neq 0$ these are highly oscillatory and not strictly positive.

Note in particular then if we choose for our $g(x)$ the form we found for the case of a single Gaussian state (2.7.17) and centre it at $X = 0$, that is we take

$$g(x) = 2^n e^{-\frac{1}{\hbar} x \cdot G x} \quad (2.7.29)$$

then

$$\chi_g(\xi) = e^{-\frac{1}{4\hbar}\xi \cdot G^{-1}\xi} \quad (2.7.30)$$

and

$$\chi_\rho(\xi) = \frac{1}{\mathcal{N}} \sum_{j,k} e^{-\frac{i}{\hbar}\xi \cdot \bar{X}_{jk}} e^{\frac{i}{2\hbar}X_k \cdot \Omega X_j} e^{-\frac{1}{4\hbar}(\xi - \Omega \delta X_{jk}) \cdot G^{-1}(\xi - \Omega \delta X_{jk})} \quad (2.7.31)$$

with

$$\rho(x) = \frac{2^n}{\mathcal{N}} \sum_k e^{-\frac{1}{\hbar}(x - X_k) \cdot G(x - X_k)} + \frac{2^n}{\mathcal{N}} \sum_{j \neq k} e^{\frac{i}{2\hbar}X_k \cdot \Omega X_j} e^{-\frac{i}{\hbar}x \cdot \Omega^T \delta X_{kj}} e^{-\frac{1}{\hbar}(x - \bar{X}_{kj}) \cdot G(x - \bar{X}_{kj})}. \quad (2.7.32)$$

2.8 Decoherence

Decoherence is often described broadly as the loss of quantum effects in the system due to interaction with an environment. In the literature decoherence is discussed in a few different ways, most commonly either in terms of the decay of a pure state to a mixed state, which is common in the physics literature, or in terms of the decay of the interference terms of the Wigner function in the phase space picture. For the first of these, it is important to note that a total superposition of the global wave function including the environment still exists, it is just the local system that appears in a mixed state.

To introduce the Wigner function indicator of decoherence it is simplest to use an example. We will consider this particular example in greater detail later in the thesis but for now we will only present a basic description of the initial state and show its time evolution.

Example 2.8.1 (Decoherence of a cat state). A cat state is in general a quantum state consisting of a linear superposition of two (or potentially more) coherent states. For the purposes of this example we will consider a superposition of two coherent states centred symmetrically

$$\psi := \frac{1}{\sqrt{2}}\psi_{y_1} + \frac{1}{\sqrt{2}}\psi_{y_2} \quad (2.8.1)$$

where ψ_{X_i} are coherent states in the form described in (2.7.3) with the covariance matrix $B = iI$, the identity matrix.

Using (2.7.32) the Wigner function of such a superposition is given by

$$\rho(x) = \frac{1}{2}\rho_{y_1}(x) + \frac{1}{2}\rho_{y_2}(x) + \frac{e^{\frac{i}{\hbar}\alpha}}{2}e^{\frac{i}{\hbar}\delta y \cdot (x - \bar{y})}\rho_{\bar{y}}(x) + \frac{e^{\frac{i}{\hbar}\alpha}}{2}e^{-\frac{i}{\hbar}\delta y \cdot (x - \bar{y})}\rho_{\bar{y}}(x) \quad (2.8.2)$$

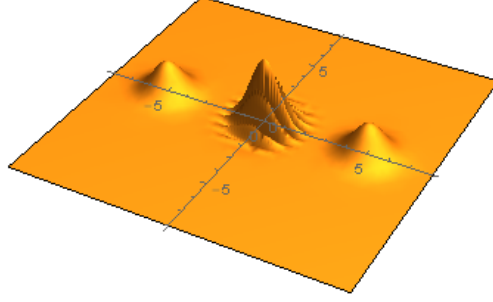
where

$$\rho_y(x) = 2^n e^{-\frac{1}{\hbar}|x - y|^2} \quad (2.8.3)$$

and we have

$$\bar{y} = \frac{1}{2}(y_1 + y_2), \quad \delta y = y_2 - y_1, \quad \alpha = \frac{1}{2}\bar{y} \cdot \begin{pmatrix} 0 & I \\ 0 & 0 \end{pmatrix} \delta y. \quad (2.8.4)$$

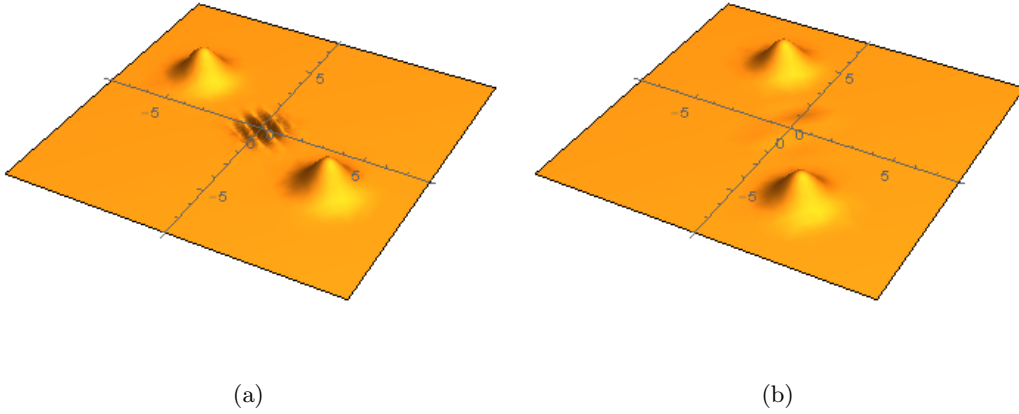
If we centre each Gaussian state symmetrically in the position axis then the Wigner function is given in Fig 2.1



(a)

Figure 2.1: A phase space picture of the Wigner function of a cat state composed of a superposition of two Gaussian coherent states centred symmetrically on the position axis at $q = \pm 5$. Note the highly oscillatory interference terms around the origin.

The main features of this Wigner function are clearly the two Gaussian peaks and the highly oscillatory interference between them. If we now evolve this state assuming interaction with a scattering environment, we see the evolution in Fig. 2.2.



(a)

(b)

Figure 2.2: A phase space picture of the evolution of the Wigner function of a cat state initially centred symmetrically on the position axis under the effects of a harmonic oscillator Hamiltonian and a scattering environment. Note how the interference in the centre rapidly decays while the Gaussian peaks broaden and rotate around the origin.

The Gaussian peaks rotate under the harmonic oscillator Hamiltonian and the interference in the middle is washed away under the influence of the environment, leaving the Wigner function consisting of two separate Gaussian peaks centred around the classical position and momentum trajectories.

We will review this example in greater detail in section 3.2 where we will show how the evolution of such a cat state under the harmonic oscillator Hamiltonian and scattering environment can be determined.

The Wigner function approach to decoherence can hence be directly seen visually and further than that, offers a direct way of quantifying the onset of decoherence in a system. Since the interference terms are characterised by highly oscillatory symbols it is natural to describe decoherence in terms of the bounding of the derivatives of these symbols by some constant. The symbol class S^0 is then the natural class to consider.

However, let us recall the the form of the equation (2.6.14),

$$\partial_t \rho = X_0 \rho + \nabla \cdot X_0 \rho + \frac{\hbar}{2} \sum_{k=1}^{2K} X_k^2 \rho. \quad (2.8.5)$$

Note that as mentioned previously, this consists of a transport term X_0 and a diffusive term $\frac{\hbar}{2} \sum_{k=1}^{2K} X_k^2$. If we compare this to the standard heat equation

$$\frac{\partial \phi}{\partial t} = D \nabla^2 \phi \quad (2.8.6)$$

where D is a diffusion constant, we see that the diffusive term $\frac{\hbar}{2} \sum_{k=1}^{2K} X_k^2$ now describes local smoothing on a scale of $\sqrt{\hbar}$. As we will see in the next chapter, if the vector fields X_0, X_j satisfy a condition from the theory of partial differential equations known as Hörmander's condition, then this local smoothing will extend to all degrees of freedom in the system. Hence we need to impose a further restriction, namely that the derivatives of ρ scale with at most $\hbar^{-\frac{1}{2}}$. This then naturally leads us to consider ρ belonging to the symbol class $S_{\frac{1}{2}}^0$.

Note that this is specific to the Lindblad equation in this form. If instead we were to consider an equation where the dispersive term had a prefactor of higher order in \hbar , or if we had higher order derivatives then we would have to adapt this definition. Since we will only be focussed on the Lindblad equation in this thesis we will not provide a more general description, but simply note that it could be extended further if necessary.

Hence we arrive at the following definition of decoherence which we will use throughout the rest of this thesis.

Definition 2.8.2. We say that a system shows *decoherence in phase space* if for any trace class $\hat{\rho}_0 \in \mathcal{T}$ the symbol $\rho_t(x)$ of the time evolved operator $\hat{\rho}_t$ is in $S_{\frac{1}{2}}^0$ for $t \geq T > 0$ uniformly. That is, for any $T > 0$ and multi-index α there exists a constant $C_{T,\alpha} > 0$ such that

$$\sup_{\substack{x \in \mathbb{R}^n \\ t \geq T}} |\partial_x^\alpha \rho_t(x)| \leq C_{T,\alpha} \hbar^{-|\alpha|/2}. \quad (2.8.7)$$

for all $\hbar \in (0, 1]$.

One might hope that that this approach to decoherence would be equivalent to the mixed state approach discussed earlier, but this is not the case. The easiest way to see why this is not true is to consider the example Lindblad equation we discussed previously describing the damping of a harmonic oscillator (2.2.5). In particular, we noted that the evolved state (2.2.62) remains pure under the Lindblad evolution,

$$\hat{\rho}_t = |\alpha_t\rangle \langle \alpha_t|. \quad (2.8.8)$$

This is not unique to this example, indeed there has been recent work in the control theory literature (see for instance [28]) where conditions for constructing desired pure states utilising the dissipation from the environment as described by the Lindblad equation are discussed. Hence, in the sense of pure and mixed states, the system would not experience decoherence.

However, as we will see in the following chapter, such a system would satisfy the Hörmander condition (3.4.2) and hence, using the main result of that chapter, namely Theorem 3.4.9, this system would satisfy (2.8.7) and hence does experience decoherence. Indeed we will consider a class of systems of this type in Chapter 4 and investigate the decoherence properties in more depth. The two approaches are thus not completely equivalent.

Because (2.8.7) provides us a concrete and testable way of determining whether a system experiences decoherence we will choose to use this approach in the rest of this thesis. It is understood that this may differ from the definition, for instance, those in the physics or quantum information literature might choose to take.

Chapter 3

Lindblad, the Hörmander condition and decoherence

3.1 Motivation and introduction

This chapter arose from work that was partly done in conjunction with Roman's summer student Jesse Parsons and is intended to be published soon. The problem we wish to consider is a simple one. Suppose we have a quantum system connected to a Markovian environment such that the Lindblad master equation applies. One of the key aspects of such system environment pairs is decoherence and characterising the rate and spread of this decoherence in the system due to the environment is of interest. This chapter will focus on using semiclassical methods to investigate decoherence via the Lindblad equation, and we will see that the fundamental condition needed to characterise decoherence is the famous Hörmander condition [20] from the theory of partial differential equations.

In the background chapter we saw that many semiclassical expansions become exact if we restrict ourselves to symbols which are at most quadratic. In particular, in (2.6.13) we saw that if we restricted ourselves to system environment pairs with $H(x)$, the symbol associated to the internal Hamiltonian, at most quadratic in $x = (q, p)$ and $L_k(x)$, the symbol associated to the k th Lindblad operators, at most linear in x , then the phase space Lindblad equation becomes an exact partial differential equation. As we saw when considering the damping of a Harmonic oscillator, such Hamiltonians and Lindblads are not uncommonly considered and hence while the results in this chapter are not truly general they do cover a wide range of systems and serve as a basis for considering more complicated systems where the full expansion of the Lindblad equation on phase space may be needed.

3.2 Solving the Lindblad equation

We start by introducing a result for the general solution of the Lindblad equation on phase space when we restrict ourselves to linear Lindblad operators and a quadratic

Hamiltonian which we will utilise in the rest of this section. Assume as before that the operators $\hat{\rho}$, \hat{H} and \hat{L}_k are given by Weyl quantizations of appropriate phase space functions $\rho(x)$, $H(x)$, $L_k(x)$ where $x = (q, p) \in \mathbb{R}^{2n}$.

Recall that we had following vector field form of the Lindblad equation for linear Lindblad operators and a quadratic Hamiltonian (see (2.6.28)):

$$\partial_t \rho = -(Ax) \cdot \nabla \rho - \text{tr}(A)\rho + \frac{\hbar}{2} \nabla \cdot M \nabla \rho. \quad (3.2.1)$$

where

$$A = F + N\Omega \quad (3.2.2)$$

for

$$F = \Omega H'' \quad (3.2.3)$$

and

$$\sum_{k=1}^K \bar{l}_k l_k^T = M + iN. \quad (3.2.4)$$

We now introduce the following theorem which in some sense goes back to Kolmogorov [29] in a special case but in the general case goes back to Kuptsov [30][31].

Theorem 3.2.1. *Define*

$$R_t := e^{tA} \quad \text{and} \quad D_t := \int_0^t R_s M R_s^T ds, \quad (3.2.5)$$

and suppose $\rho(t, x)$ is a solution to the Lindblad equation (2.6.28) with initial condition $\rho(0, x) = \rho_0(x) \in L^1(\mathbb{R}^{2n})$. Then for $t \geq 0$ we have

$$\chi(t, \xi) = \chi_0(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi}. \quad (3.2.6)$$

Furthermore, if D_t is nonsingular, then $\rho(t, x)$ satisfies

$$\rho(t, R_t x) |\det R_t| = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} K_\hbar(t, y) \rho_0(x + y) dy, \quad (3.2.7)$$

with the kernel

$$K_\hbar(t, y) = \frac{1}{\sqrt{\det C_t}} e^{-\frac{1}{2\hbar} y \cdot C_t^{-1} y} \quad (3.2.8)$$

where we defined

$$C_t = R_{-t} D_t R_{-t}^T = \int_0^t R_{-s} M R_{-s}^T ds. \quad (3.2.9)$$

Proof. We start from

$$\partial_t \rho = -(Ax) \cdot \nabla \rho - \text{tr}(A)\rho + \frac{\hbar}{2} \nabla \cdot M \nabla \rho. \quad (3.2.10)$$

CHAPTER 3. LINDBLAD, THE HÖRMANDER CONDITION AND DECOHERENCE

Taking the Fourier transform to get the characteristic function we arrive at the following:

$$\partial_t \chi(t, \xi) = (A^T \xi) \cdot \nabla_\xi \chi(t, \xi) - \frac{1}{2\hbar} \xi \cdot M \xi \chi(t, \xi). \quad (3.2.11)$$

If we make an ansatz in the form claimed:

$$\chi(t, \xi) = \chi_0(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} \quad (3.2.12)$$

where R_t and D_t are $2n \times 2n$ matrices and we take D_t symmetric with initial conditions $R_0 = I$ and $D_0 = 0$ then we have on the LHS:

$$(\partial_t R_t^T \xi) \cdot (\nabla \chi_0)(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} - \frac{1}{2\hbar} \xi \cdot \partial_t D_t \xi \chi(t, \xi). \quad (3.2.13)$$

while on the RHS we have

$$(A^T \xi) \cdot (R_t \nabla \chi_0)(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} - \frac{1}{\hbar} (A^T \xi) \cdot D_t \xi \chi(t, \xi) - \frac{1}{2\hbar} \xi \cdot M \xi \chi(t, \xi). \quad (3.2.14)$$

Rearranging

$$(A^T \xi) \cdot D_t \xi = \xi \cdot A D_t \xi = \frac{1}{2} \xi \cdot (A D_t + D_t A^T) \xi \quad (3.2.15)$$

we obtain upon comparison the following relations:

$$\partial_t R_t = A R_t, \quad (3.2.16)$$

$$\partial_t D_t = A D_t + D_t A^T + M. \quad (3.2.17)$$

We can solve the first equation with $R_t = e^{tA}$ and the second can be solved by taking $D_t = \int_0^t R_s M R_s^T ds$ which can be seen directly from

$$A D_t + D_t A^T + M = \int_0^t \frac{d}{ds} (R_s M R_s^T) ds = R_t M R_t^T = \partial_t D_t. \quad (3.2.18)$$

Due to the uniqueness of solutions to the initial value problem this completes the first part of the proof.

By taking the inverse Fourier transform and inserting $\chi_0(\xi) = \int e^{-\frac{i}{\hbar} y \cdot \xi} \rho_0(y) dy$ we get that

$$\begin{aligned} \rho(t, x) &= \frac{1}{(2\pi\hbar)^{2n}} \int \int \rho_0 e^{\frac{i}{\hbar} (x - R_t y) \cdot \xi} e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} dy d\xi \\ &= \frac{1}{(2\pi\hbar)^n \sqrt{\det D_t}} \int \rho_0(y) e^{-\frac{1}{2\hbar} (x - R_t y) \cdot D_t^{-1} (x - R_t y)} dy. \end{aligned} \quad (3.2.19)$$

Here we have performed the ξ integral which is allowed as long as D_t is non-singular. \square

Remark 3.2.2.

- If we were considering classical mechanics, ρ would be analogous to a probability density, and as a result it would be very natural to consider the density $\rho(t, x)|dx|$. Hence, if we compose with R_t , it becomes similarly natural to consider the density $\rho(t, R_t x)|\det R_t||dx|$.
- As we can see, the solution (3.2.6), and hence the time evolution of $\rho(t, x)$, is characterised entirely by the two matrices R_t and D_t . Indeed, if we consider (3.2.7) with the Kernel defined by (3.2.8) we see that for non-degenerate D_t , the time evolution is given by a transport part described by R_t^{-1} and a diffusive part on a scale of $\frac{\sqrt{\hbar}}{\|D_t\|}$. This diffusive part will average out rapid oscillations and hence describes the onset of decoherence in the system.
- Notice that $K_h(t, y) > 0$ and further $\int_{\mathbb{R}^{2n}} K_h(t, y) dy = 1$. This implies that

$$\int_{\mathbb{R}^{2n}} \rho(t, x) dx = \int_{\mathbb{R}^{2n}} \rho_0(x) dx, \quad (3.2.20)$$

and also that $\rho(t, x) > 0$ for $t > 0$ if our initial $\rho_0(x) \geq 0$.

- Note that in the case where our Lindblad terms are zero, M and N are zero, and hence D_t is zero and R_t is simply

$$R_t = e^{tF} \quad (3.2.21)$$

which is just the matrix $S(t)$ we discussed in Section 2.3.3.

Let us give some examples of R_t and D_t in systems with one degree of freedom.

Example 3.2.3 (One degree of freedom: a cloud of dust scatterers). First let us consider what is possibly the simplest environment we can have, a cloud of dust scatterers defined by a single Lindblad operator given as the quantization of the symbol $L = \sqrt{\sigma}q$. In this case we have that, writing $L = x \cdot \Omega l$ as above, $l = \begin{pmatrix} 0 \\ \sqrt{\sigma} \end{pmatrix}$ and using (2.6.26) we hence have

$$N = 0, \quad M = \begin{pmatrix} 0 \\ \sqrt{\sigma} \end{pmatrix} \begin{pmatrix} 0 & \sqrt{\sigma} \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & \sigma \end{pmatrix}. \quad (3.2.22)$$

Immediately then $A = F + N\Omega = F$ and hence

$$R_t = e^{tF}. \quad (3.2.23)$$

From this we find that

$$D_t = \int_0^t e^{sF} \begin{pmatrix} 0 & 0 \\ 0 & \sigma \end{pmatrix} e^{sF^T} ds = \sigma \int_0^t e_2(s) e_2(s)^T ds \quad (3.2.24)$$

where we have defined $e_2(s) = R_s e_2$ for e_2 the standard second basis vector. Lets now consider some simple systems:

(i) Let $H(q, p) = \frac{\omega}{2}aa^\dagger = \frac{\omega}{2}(q^2 + p^2)$, then $H'' = \begin{pmatrix} \omega & 0 \\ 0 & \omega \end{pmatrix}$ and thus $F = \omega\Omega$ and hence

$$R_t = e^{tF} = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) \\ -\sin(\omega t) & \cos(\omega t) \end{pmatrix}, \quad (3.2.25)$$

the standard rotation matrix. Hence we have that

$$e_2(s) = \begin{pmatrix} \sin \omega s \\ \cos \omega s \end{pmatrix} \quad (3.2.26)$$

and therefore

$$\begin{aligned} D_t &= \sigma \int_0^t \begin{pmatrix} \sin^2 \omega s & \sin \omega s \cos \omega s \\ \sin \omega s \cos \omega s & \cos^2 \omega s \end{pmatrix} ds \\ &= \frac{\sigma t}{2} I + \frac{\sigma}{2\omega} \begin{pmatrix} -\sin \omega t \cos \omega t & \sin^2 \omega t \\ \sin^2 \omega t & \sin \omega t \cos \omega t \end{pmatrix}. \end{aligned} \quad (3.2.27)$$

(ii) Let $H(q, p) = \frac{1}{2}p^2$, i.e. the free particle. Then,

$$R_t = \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix}. \quad (3.2.28)$$

Thus $e_2(s) = \begin{pmatrix} s \\ 1 \end{pmatrix}$ and we find

$$D_t = \sigma \int_0^t \begin{pmatrix} s^2 & s \\ s & 1 \end{pmatrix} ds = \sigma \begin{pmatrix} \frac{t^3}{3} & \frac{t^2}{2} \\ \frac{t^2}{2} & t \end{pmatrix}. \quad (3.2.29)$$

(iii) Finally let us consider the hyperbolic Hamiltonian $H(q, p) = \lambda qp$ for $\lambda > 0$. Then

$$R_t = \begin{pmatrix} e^{\lambda t} & 0 \\ 0 & e^{-\lambda t} \end{pmatrix}. \quad (3.2.30)$$

Thus,

$$D_t = \sigma \int_0^t \begin{pmatrix} 0 & 0 \\ 0 & e^{-2\lambda s} \end{pmatrix} ds = \frac{\sigma}{2\lambda} (1 - e^{-2\lambda t}) \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \quad (3.2.31)$$

Example 3.2.4 (One degree of freedom: a heat bath). Let us now consider an environment described by a simple Heat bath. In this case we have two Lindblad operators given by, for $\mu > \lambda > 0$

$$L_c = \gamma a = \gamma(q - ip), \quad L_a = \mu a^\dagger = \mu(q + ip), \quad (3.2.32)$$

which are the creation and annihilation operators respectively. Recall that the temperature of the bath was related to the logarithm of the ratio $\beta = \frac{2}{\omega\hbar} \ln\left(\frac{\mu}{\gamma}\right)$ in the case of the harmonic oscillator Hamiltonian. Proceeding as before we find that

$$l_c = \gamma \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad l_a = \mu \begin{pmatrix} -i \\ 1 \end{pmatrix} \quad (3.2.33)$$

and hence

$$N = (\mu^2 - \gamma^2)\Omega \quad (3.2.34)$$

and

$$M = (\mu^2 + \gamma^2)I. \quad (3.2.35)$$

Hence we find that

$$A = F - (\mu^2 - \gamma^2)I \quad (3.2.36)$$

and hence

$$R_t = e^{-(\mu^2 - \gamma^2)t} e^{tF}. \quad (3.2.37)$$

We then find immediately that

$$D_t = (\mu^2 + \gamma^2) \int_0^t e^{-2(\mu^2 - \gamma^2)s} e^{sF} e^{sF^T} ds. \quad (3.2.38)$$

Lets now consider the same examples as in the scattering case.

(i) For $H(q, p) = \frac{\omega}{2} aa^\dagger = \frac{\omega}{2}(q^2 + p^2)$ we have as before

$$e^{tF} = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) \\ -\sin(\omega t) & \cos(\omega t) \end{pmatrix} \quad (3.2.39)$$

and hence

$$R_t = e^{-(\mu^2 - \gamma^2)t} \begin{pmatrix} \cos(\omega t) & \sin(\omega t) \\ -\sin(\omega t) & \cos(\omega t) \end{pmatrix}. \quad (3.2.40)$$

As the multiplication of a rotation matrix with its transpose is the identity, we have

$$D_t = (\mu^2 + \gamma^2) \left(\int_0^t e^{-2(\mu^2 - \gamma^2)s} ds \right) I \quad (3.2.41)$$

$$= \frac{1}{2} \frac{\mu^2 + \gamma^2}{\mu^2 - \gamma^2} \left(1 - e^{-2(\mu^2 - \gamma^2)t} \right) I. \quad (3.2.42)$$

(ii) For $H(q, p) = \frac{1}{2}p^2$ we have $e^{tF} = \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix}$ and thus

$$R_t = e^{-(\mu^2 - \gamma^2)t} \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \quad (3.2.43)$$

and hence

$$D_t = (\mu^2 + \gamma^2) \int_0^t e^{-2(\mu^2 - \gamma^2)s} \begin{pmatrix} 1 + s^2 & s \\ s & 1 \end{pmatrix} ds. \quad (3.2.44)$$

(iii) For $H(q, p) = \lambda qp$, $\lambda > 0$ then

$$R_t = e^{-(\mu^2 - \gamma^2)t} \begin{pmatrix} e^{\lambda t} & 0 \\ 0 & e^{-\lambda t} \end{pmatrix} \quad (3.2.45)$$

and

$$D_t = (\mu^2 + \gamma^2) \int_0^t \begin{pmatrix} e^{-2(\mu^2 - \gamma^2 + \lambda)s} & 0 \\ 0 & e^{-2(\mu^2 - \gamma^2 - \lambda)s} \end{pmatrix} ds \quad (3.2.46)$$

which, if we define $\alpha = \mu^2 + \gamma^2$, $\alpha_{\pm} = 2(\mu^2 - \gamma^2 \pm \lambda)$, is given by

$$D_t = \begin{pmatrix} \frac{\alpha}{\alpha_+}(1 - e^{-\alpha_+ t}) & 0 \\ 0 & \frac{\alpha}{\alpha_-}(1 - e^{-\alpha_- t}) \end{pmatrix}. \quad (3.2.47)$$

As discussed in the previous chapter, coherent states are a very useful set of example states to consider, in particular because they can be used to construct any more complex state as well as closely following the classical trajectories. Because of this, let's consider the Weyl symbols of coherent states in the next Lemma.

Lemma 3.2.5. *Let ψ_0 be a coherent states centred at $y = 0$ with an associated (Gaussian) characteristic function*

$$\chi_0(\xi) = e^{-\frac{1}{4\hbar}\xi \cdot G^{-1}\xi}. \quad (3.2.48)$$

The time evolution of the coherent state

$$\psi = \frac{1}{\sqrt{N}} \sum_{j=1}^N T_{\Omega}(y_j) \psi_0 \quad (3.2.49)$$

has Weyl symbol

$$\rho(t, x) = \frac{1}{N} \sum_{j,k=1}^N \rho_{jk}(t, x) \quad (3.2.50)$$

where the individual $\rho_{jk}(t, x)$ are given by

$$\rho_{jk}(t, x) = 2^n e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} \sqrt{\det G_t} e^{-\frac{1}{2\hbar} (\Omega \delta y_{jk}) \cdot \tilde{C}_t (\Omega \delta y_{jk})} e^{\frac{i}{\hbar} \xi_{jk}(t) \cdot (x - \bar{y}_{jk}(t))} e^{-\frac{1}{\hbar} (x - \bar{y}_{jk}(t)) \cdot G_t (x - \bar{y}_{jk}(t))} \quad (3.2.51)$$

where

$$\bar{y}_{jk}(t) = R_t \bar{y}_{jk}, \quad (3.2.52)$$

$$G_t := ([R_{-t}^T G R_{-t}]^{-1} + 2D_t)^{-1}, \quad (3.2.53)$$

$$\tilde{C}_t := C_t (I + 2GC_t)^{-1}, \quad (3.2.54)$$

and

$$\xi_{jk}(t) := R_{-t}^T (I + 2GC_t)^{-1} (\Omega \delta y_{jk}) \quad (3.2.55)$$

with $\bar{y}_{jk} = \frac{1}{2}(y_j + y_k)$ and $\delta y_{jk} = y_j - y_k$.

3.2. SOLVING THE LINDBLAD EQUATION

Proof. Note that $\rho_{jk}(0, x)$ has, using the result (2.7.31), characteristic function

$$\chi_{jk}(0, \xi) = e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} e^{-\frac{i}{\hbar} \xi \cdot \bar{y}_{jk}} e^{-\frac{1}{4\hbar} (\xi - \Omega \delta y_{jk}) \cdot G^{-1} (\xi - \Omega \delta y_{jk})}. \quad (3.2.56)$$

Then, using Theorem 3.2.1 we have that

$$\chi_{jk}(t, \xi) = \chi_{jk}(0, R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi}. \quad (3.2.57)$$

Expanding $\chi_{jk}(0, R_t^T \xi)$ we have

$$\begin{aligned} \chi_{jk}(0, R_t^T \xi) &= e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} e^{-\frac{i}{\hbar} (R_t^T \xi) \cdot \bar{y}_{jk}} e^{-\frac{1}{4\hbar} (R_t^T \xi - \Omega \delta y_{jk}) \cdot G^{-1} (R_t^T \xi - \Omega \delta y_{jk})} \\ &= e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} e^{-\frac{i}{\hbar} \xi \cdot R_t \bar{y}_{jk}} e^{-\frac{1}{4\hbar} (\xi - R_{-t}^T \Omega \delta y_{jk}) \cdot R_t G^{-1} R_t^T (\xi - R_{-t}^T \Omega \delta y_{jk})} \\ &= e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} e^{-\frac{i}{\hbar} \xi \cdot \bar{y}_{jk}(t)} e^{-\frac{1}{4\hbar} (\xi - \delta \xi) \cdot [R_{-t}^T G^{-1} R_{-t}]^{-1} (\xi - \delta \xi)} \end{aligned}$$

where we have defined

$$\bar{y}_{jk}(t) = R_t \bar{y}_{jk}, \quad \delta \xi = R_{-t}^T \Omega \delta y_{jk}. \quad (3.2.58)$$

Hence we have that

$$\chi_{jk}(t, \xi) = e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} e^{-\frac{i}{\hbar} \xi \cdot \bar{y}_{jk}(t)} e^{-\frac{1}{4\hbar} (\xi - \delta \xi) \cdot [R_{-t}^T G^{-1} R_{-t}]^{-1} (\xi - \delta \xi)} e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi}. \quad (3.2.59)$$

To find the Weyl symbol, we take the inverse Fourier transform

$$\begin{aligned} \rho_{jk}(t, x) &= \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} \xi \cdot x} \chi_{jk}(t, \xi) d\xi \\ &= \frac{e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j}}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} \xi \cdot (x - \bar{y}_{jk}(t))} e^{-\frac{1}{4\hbar} (\xi - \delta \xi) \cdot [R_{-t}^T G^{-1} R_{-t}]^{-1} (\xi - \delta \xi)} e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} d\xi. \end{aligned}$$

If we define

$$x_t = x - \bar{y}_{jk}(t) \quad (3.2.60)$$

then we find ourselves in the situation of (A.0.1).

$$\rho_{jk}(t, x) = e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} I(x_t, \delta \xi, \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1}, D_t) \quad (3.2.61)$$

and applying the lemma we have

$$\begin{aligned} \rho_{jk}(t, x) &= \frac{e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j}}{\sqrt{\det(D_t + \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1})}} \\ &\quad \times e^{-\frac{1}{2\hbar} \delta \xi \cdot (D_t + \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1})^{-1} \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1} \delta \xi} \\ &\quad \times e^{\frac{i}{\hbar} \delta \xi \cdot \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1} (D_t + \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1})^{-1} x_t} \\ &\quad \times e^{-\frac{1}{2\hbar} x_t \cdot (D_t + \frac{1}{2} [R_{-t}^T G^{-1} R_{-t}]^{-1})^{-1} x_t}. \end{aligned}$$

Now lets define as stated

$$G_t = (2D_t + [R_{-t}^T G^{-1} R_{-t}]^{-1})^{-1}. \quad (3.2.62)$$

Then we can write

$$\begin{aligned} \rho_{jk}(t, x) &= \frac{e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j}}{\sqrt{\det(\frac{1}{2} G_t^{-1})}} \\ &\times e^{-\frac{1}{2\hbar} \delta \xi \cdot (D_t G_t [R_{-t}^T G^{-1} R_{-t}]^{-1}) \delta \xi} \\ &\times e^{\frac{i}{\hbar} \delta \xi \cdot ([R_{-t}^T G^{-1} R_{-t}]^{-1} G_t) x_t} \\ &\times e^{-\frac{1}{\hbar} x_t \cdot G_t x_t}. \end{aligned}$$

We now look to simplify the objects $G_t [R_{-t}^T G^{-1} R_{-t}]^{-1}$ and $[R_{-t}^T G^{-1} R_{-t}]^{-1} G_t$, we have that

$$\begin{aligned} G_t [R_{-t}^T G^{-1} R_{-t}]^{-1} &= (2D_t + [R_{-t}^T G^{-1} R_{-t}]^{-1})^{-1} [R_{-t}^T G^{-1} R_{-t}]^{-1} \\ &= (I + 2[R_{-t}^T G^{-1} R_{-t}] D_t)^{-1} \\ &= (R_{-t}^T R_t^T + 2R_{-t}^T G^{-1} R_{-t} D_t R_{-t}^T R_t^T)^{-1} \\ &= (R_{-t}^T (I + 2G R_{-t} D_t R_{-t}^T) R_t^T)^{-1} \\ &= R_{-t}^T (I + 2G C_t)^{-1} R_t^T \end{aligned}$$

where in the last line we have used the definition of C_t (3.2.9). If we do the same for the second combination we similarly get

$$[R_{-t}^T G^{-1} R_{-t}]^{-1} G_t = R_t (I + 2C_t G)^{-1} R_{-t}. \quad (3.2.63)$$

We now have

$$\begin{aligned} \rho_{jk}(t, x) &= 2^n e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} \sqrt{\det(G_t)} \\ &\times e^{-\frac{1}{2\hbar} \delta \xi \cdot D_t R_{-t}^T (I + 2G C_t)^{-1} R_t^T \delta \xi} \\ &\times e^{\frac{i}{\hbar} \delta \xi \cdot R_t (I + 2C_t G)^{-1} R_{-t} x_t} \\ &\times e^{-\frac{1}{\hbar} x_t \cdot G_t x_t}. \end{aligned}$$

Now, we re-expand $\delta \xi = R_{-t}^T \Omega \delta y_{jk}$ to get

$$\begin{aligned} \rho_{jk}(t, x) &= 2^n e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} \sqrt{\det(G_t)} \\ &\times e^{-\frac{1}{2\hbar} (\Omega \delta y_{jk}) \cdot R_{-t} D_t R_{-t}^T (I + 2G C_t)^{-1} R_{-t}^T R_t^T (\Omega \delta y_{jk})} \\ &\times e^{\frac{i}{\hbar} (\Omega \delta y_{jk}) \cdot R_{-t} R_t (I + 2C_t G)^{-1} R_{-t} x_t} \\ &\times e^{-\frac{1}{\hbar} x_t \cdot G_t x_t}. \end{aligned}$$

Again, using the definition of C_t (3.2.9) and now also defining

$$\tilde{C}_t := C_t (I + 2GC_t)^{-1} \quad (3.2.64)$$

as well as

$$\xi_{jk}(t) := R_{-t}^T (I + 2C_t G)^{-T} (\Omega \delta y_{jk}) \quad (3.2.65)$$

$$= R_{-t}^T (I + 2GC_t)^{-1} (\Omega \delta y_{jk}) \quad (3.2.66)$$

since I , G and C_t are all symmetric, then we have finally that

$$\rho_{jk}(t, x) = 2^n e^{\frac{i}{2\hbar} y_k \cdot \Omega y_j} \sqrt{\det(G_t)} e^{-\frac{1}{2\hbar} (\Omega \delta y_{jk}) \cdot \tilde{C}_t (\Omega \delta y_{jk})} e^{\frac{i}{\hbar} \xi_{jk}(t) \cdot (x - \bar{y}_{jk}(t))} e^{-\frac{1}{\hbar} (x - \bar{y}_{jk}(t)) \cdot G_t (x - \bar{y}_{jk}(t))}.$$

where we have re-expanded $x_t = x - \bar{y}_{jk}(t)$. \square

Note that if we consider only the diagonal terms for which $j = k$, then $\delta y_{jk} = \delta y_{jj} = 0$ and as a result $\rho_{jj}(t, x)$ reduces simply to

$$\rho_{jj}(t, x) = 2^n \sqrt{\det G_t} e^{-\frac{1}{\hbar} (x - y_j(t)) \cdot G_t (x - y_j(t))} \quad (3.2.67)$$

where we have defined $y_j(t) = \bar{y}_{jj}(t) = R_t y_j$. If we compare this to (2.7.5) we see that this is of the form of a Wigner function of a Gaussian state centred at $y_j(t)$ with covariance matrix given by G_t . These diagonal terms can hence be thought of as describing how the original individual Gaussian states evolve in time, and in particular they closely follow the classical trajectories of the system.

The cross terms where $j \neq k$ are where the interesting quantum superpositions appear. These terms are no longer purely Gaussian and instead are highly oscillatory. This is a purely quantum phenomena and is a signifier of quantum coherence. Decoherence is then signified by the decay of these terms and increasing localization of the full state around the individual Gaussian states described by the diagonal terms. Hence we are interested in the *size* of the cross components ρ_{jk} for $j \neq k$, the expectation being that we should see rapid damping in time when the system is coupled to an environment inducing decoherence. We now present some estimates which will allow us to quantify this damping.

Lemma 3.2.6. *Suppose that for an initial state $\hat{\rho}_0$ the characteristic function satisfies*

$$|\chi_0(\xi)| = e^{-\frac{1}{4\hbar} (\xi - \Omega \delta y) \cdot G^{-1} (\xi - \Omega \delta y)} \quad (3.2.68)$$

where the matrix G is positive definite. Then the Hilbert-Schmidt norm of the time-evolved state ρ_t satisfies

$$\|\hat{\rho}_t\|_{HS}^2 = \frac{|\det R_{-t}| \sqrt{\det G}}{\sqrt{\det(I + 2GC_t)}} e^{-\frac{1}{\hbar} \Omega \delta y \cdot \tilde{C}_t \Omega \delta y} \quad (3.2.69)$$

with

$$\tilde{C}_t = C_t (I + 2GC_t)^{-1}. \quad (3.2.70)$$

We also have that

$$|\rho(t, x)| \leq \frac{2^n |\det R_{-t}| \sqrt{\det G}}{\sqrt{\det(I + 2GC_t)}} e^{-\frac{1}{2\hbar} \Omega \delta y \cdot \tilde{C}_t \Omega \delta y}. \quad (3.2.71)$$

Proof. We use the result from the background chapter (2.5.14) that the norm of an operator given as the quantization of an L^2 symbol is proportional to the L^2 norm of the symbol. We have that

$$\|\hat{\rho}_t\|_{\text{HS}} = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} |\rho(t, x)|^2 dx = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} |\chi(t, \xi)|^2 d\xi \quad (3.2.72)$$

with the second equality simply being Plancherel's theorem [42]. Then, inserting the result of Theorem 3.2.1 for the characteristic function of the time evolved density operator we have

$$\begin{aligned} \|\hat{\rho}_t\|_{\text{HS}}^2 &= \frac{1}{(2\pi\hbar)^n} \int |\chi_0(R_t^T \xi)|^2 e^{-\frac{1}{\hbar} \xi \cdot D_t \xi} d\xi \\ &= \frac{|\det R_{-t}|}{(2\pi\hbar)^n} \int |\chi_0(\xi)|^2 e^{-\frac{1}{\hbar} \xi \cdot C_t \xi} d\xi \\ &= \frac{|\det R_{-t}|}{(2\pi\hbar)^n} \int e^{-\frac{1}{2\hbar} (\xi - \Omega \delta y) \cdot G^{-1} (\xi - \Omega \delta y)} e^{-\frac{1}{\hbar} \xi \cdot C_t \xi} d\xi. \end{aligned} \quad (3.2.73)$$

Here we have relabelled $\xi \rightarrow R_t^T \xi$ and used that $C_t = R_{-t} D_t R_{-t}^T$ noting that $R_t^{-1} = R_{-t}$. If we define $\delta\xi = \Omega \delta y_{jk}$ then we are left with the integral

$$\|\hat{\rho}_t\|_{\text{HS}}^2 = \frac{|\det R_{-t}|}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} e^{-\frac{1}{2\hbar} (\xi - \delta\xi) \cdot G^{-1} (\xi - \delta\xi)} e^{-\frac{1}{\hbar} \xi \cdot C_t \xi} d\xi. \quad (3.2.74)$$

Note then that, up to the prefactor of $|\det R_{-t}|$, this is simply a special case of our Gaussian integral lemma (A.0.1) described in the appendix with $x = 0$, $\mathcal{A} = G^{-1}$ and $\mathcal{B} = 2C_t$. If we use these in the result we have

$$\begin{aligned} \|\hat{\rho}_t\|_{\text{HS}}^2 &= |\det R_{-t}| I(0, \delta\xi, G^{-1}, 2C_t) \\ &= \frac{|\det R_{-t}|}{\sqrt{\det(G^{-1} + 2C_t)}} e^{-\frac{1}{2\hbar} \delta\xi \cdot (2C_t(G^{-1} + 2C_t)^{-1} G^{-1}) \delta\xi} \\ &= \frac{|\det R_{-t}| \sqrt{\det G}}{\sqrt{\det(I + 2GC_t)}} e^{-\frac{1}{\hbar} \delta\xi \cdot (C_t(I + 2GC_t)^{-1} G G^{-1}) \delta\xi} \\ &= \frac{|\det R_{-t}| \sqrt{\det G}}{\sqrt{\det(I + 2GC_t)}} e^{-\frac{1}{\hbar} \delta\xi \cdot \tilde{C}_t \delta\xi} \end{aligned}$$

Recalling $\delta\xi = \Omega \delta y$ we get the first result (3.2.69).

For the second result, note that, since $\rho(t, x)$ is simply the inverse Fourier transform of $\chi(t, \xi)$ (see (2.5.20)), we have that

$$|\rho(t, x)| = \frac{1}{(2\pi\hbar)^n} \left| \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} x \cdot \xi} \chi(t, \xi) d\xi \right| \leq \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} |\chi(t, \xi)| d\xi. \quad (3.2.75)$$

From here the same method is used as for the previous calculation. Inserting the result of Theorem 3.2.1 and expanding we have that

$$|\rho(t, x)| \leq \frac{|\det R_{-t}|}{(2\pi\hbar)^n} \int e^{-\frac{1}{4\hbar}(\xi - \delta\xi) \cdot G^{-1}(\xi - \delta\xi)} e^{-\frac{1}{2\hbar}\xi \cdot C_t \xi} d\xi. \quad (3.2.76)$$

Now using (A.0.1) as above but with $\mathcal{A} = \frac{1}{2}G^{-1}$ and $\mathcal{B} = C_t$ this time we get in the same way

$$|\rho(t, x)| \leq \frac{2^n |\det R_{-t}| \sqrt{\det G}}{\sqrt{\det(I + 2GC_t)}} e^{-\frac{1}{2\hbar}\delta\xi \cdot \tilde{C}_t \delta\xi} \quad (3.2.77)$$

which upon taking $\delta\xi = \Omega\delta y$ gives the result (3.2.71). \square

Lets now give some examples, again restricting ourselves to the one dimensional case $n = 1$ and in particular revisiting the scattering environment.

Example 3.2.7 (A cat state: Harmonic Oscillator and Scattering environment). We begin by revisiting the example we briefly discussed when introducing the concept of decoherence in the background chapter (2.8.1), and now we can be more explicit with how we arrived at time evolution.

We consider a initial cat state $|\psi(0)\rangle$ defined as the normalized sum of two coherent states $|\psi_{y_j}^B\rangle$ of the form (2.7.3)

$$|\psi(0)\rangle = \frac{1}{\sqrt{2}} (|\psi_{y_1}^B(0)\rangle + |\psi_{y_2}^B(0)\rangle). \quad (3.2.78)$$

We have an internal harmonic oscillator Hamiltonian given as the quantization of $H(x) = \frac{\omega}{2}aa^\dagger = \frac{\omega}{2}(q^2 + p^2)$ and a single Lindblad operator describing a scattering environment given by $L(x) = \sqrt{\sigma}q$.

We saw from Theorem 3.2.1 that the time evolution of the symbol $\rho(t, x)$ of the density operator is determined entirely by the matrices R_t and D_t and we even computed these directly in the one dimensional case in Example (3.2.3) as

$$R_t = \begin{pmatrix} \cos(\omega t) & \sin(\omega t) \\ -\sin(\omega t) & \cos(\omega t) \end{pmatrix}, \quad (3.2.79)$$

and

$$D_t = \frac{\sigma t}{2}I + \frac{\sigma}{2\omega} \begin{pmatrix} -\sin \omega t \cos \omega t & \sin^2 \omega t \\ \sin^2 \omega t & \sin \omega t \cos \omega t \end{pmatrix}. \quad (3.2.80)$$

Given this, we can either use Theorem 3.2.1 directly and compute the characteristic function and then perform the inverse Fourier transform, or we can use Lemma 3.2.5.

Let's choose the simplest possible cat state we can, in particular lets let the matrix $B = iI$ for the individual coherent states. In this case, the initial matrix $G = G_0 = I$ (2.7.6). Since our R_t is simply a rotation matrix and hence $R_t^T = R_{-t}$ we find that, recalling $C_t = R_{-t}D_tR_{-t}^T$,

$$G_t = (I + 2D_t)^{-1}, \quad (3.2.81)$$

$$\tilde{C}_t = C_t(I + 2C_t)^{-1} = R_{-t}D_t(I + 2D_t)^{-1}R_t, \quad (3.2.82)$$

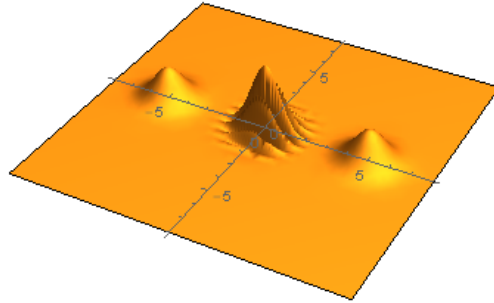
and

$$\xi_{jk}(t) = R_{-t}^T(I + 2C_t)^{-1}(\Omega\delta y_{jk}) = (I + 2D_t)^{-1}R_t(\Omega\delta y_{jk}). \quad (3.2.83)$$

Let's use these to find the time evolution of our cat state. In what follows we work in units where $\hbar = 1$ and we consider a cat state with coherent states symmetrically placed on the q axis at

$$y_1 = \begin{pmatrix} 5 \\ 0 \end{pmatrix}, \quad y_2 = \begin{pmatrix} -5 \\ 0 \end{pmatrix}. \quad (3.2.84)$$

For the internal harmonic oscillator Hamiltonian we take a frequency $\omega = 1$ and a scattering strength of $\sigma = 0.1$. The Weyl symbol ρ of the initial cat state is shown in Fig. 3.1 and is characterised by two Gaussian peaks centred around the points y_1 and y_2 in phase space and a highly oscillatory interference regime around the origin.



(a) $t = 0$

Figure 3.1: $\rho(0, x)$ for a cat state composed of a superposition of two Gaussian coherent states centred symmetrically on the position axis at $q = \pm 5$. Note the highly oscillatory interference terms around the origin.

If we now use Lemma (3.2.5) to determine $\rho(t, x)$ we find that, as we would expect, the two Gaussian peaks rotate around the origin due to the internal harmonic oscillator Hamiltonian, but also the interference terms around the origin are rapidly damped away due to the influence of the scattering environment, as shown in Fig. 3.2.

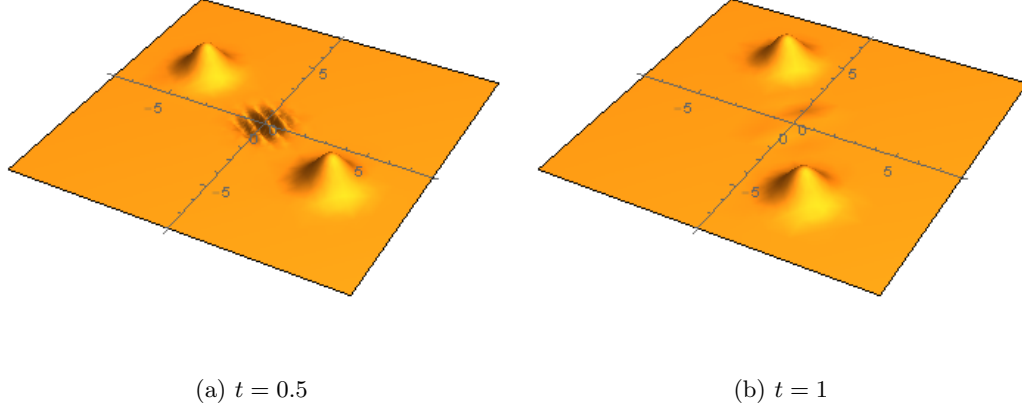


Figure 3.2: $\rho(t, x)$ for cat state initially centred symmetrically on the position axis under the effects of a harmonic oscillator Hamiltonian and a scattering environment. Note how the interference in the centre rapidly decays while the Gaussian peaks broaden and rotate around the origin.

If we wish to quantify the speed of this decay, we can use Lemma 3.2.6 to determine the Hilbert schmidt norm of each of the 4 terms in the sum (3.2.50) as shown in Fig. 3.3.

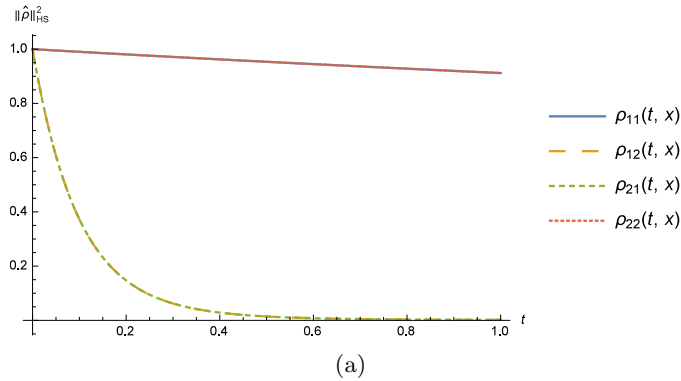


Figure 3.3: The Hilbert-Schmidt norm for each of the individual $\rho_{jk}(t, x)$ in Lemma 3.2.6 for a harmonic oscillator Hamiltonian and a scattering environment initialised on the q -axis. Note that the cross terms $j \neq k$ decay much more rapidly.

The cross terms ρ_{12} and ρ_{21} decay much more rapidly than the diagonal terms, this is an indicator of decoherence and the increased localization around the classical trajectories. Note that there is an overall decay of *all* terms arising from the prefactor $\left(\sqrt{\det(I + 2GC_t)}\right)^{-1}$ but it is much slower.

Let us make a very simple change to our initial state, so that instead of the two Gaussians being symmetrically placed on the q -axis, they are instead placed on the p -axis at

$$y_1 = \begin{pmatrix} 0 \\ 5 \end{pmatrix}, \quad y_2 = \begin{pmatrix} 0 \\ -5 \end{pmatrix}. \quad (3.2.85)$$

In this case the evolution of $\rho(t, x)$ looks roughly the same, but the *rate* of the decay of the cross terms is much slower. Indeed, if we compute the Hilbert-Schmidt norm as we did above, we see this clearly in Fig. 3.4

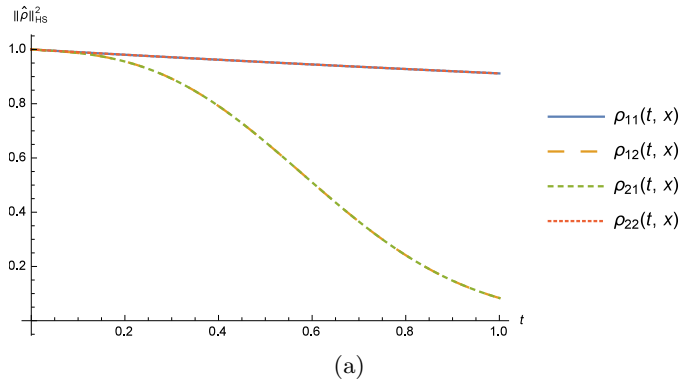


Figure 3.4: The Hilbert-Schmidt norm for each of the individual $\rho_{jk}(t, x)$ in Lemma 3.2.6 for a harmonic oscillator Hamiltonian and a scattering environment initialised on the p -axis. Note that the cross terms $j \neq k$ decay much more rapidly than the diagonal terms, but far slower than the in the q initialised case.

Example 3.2.8 (A cat state: Hyperbolic Hamiltonian and Scattering environment). Now lets revisit another of the examples we considered already in (3.2.3), namely the example of a Hyperbolic Hamiltonian $H(x) = \lambda qp$. We can proceed as in the previous example and apply the results of Lemma 3.2.5 to determine the Weyl symbol $\rho(t, x)$. If we take $\lambda = 1$ and similar to the above example take $\sigma = 0.1$, and we place our coherent states symmetrically on the q axis at

$$y_1 = \begin{pmatrix} 5 \\ 0 \end{pmatrix}, \quad y_2 = \begin{pmatrix} -5 \\ 0 \end{pmatrix}. \quad (3.2.86)$$

we find that the initial state is again given by Fig. 3.1. If we now evolve the system, we find that instead of rotating around the centre, the coherent states travel linearly away from each other along the q axis as shown in Fig. 3.5.

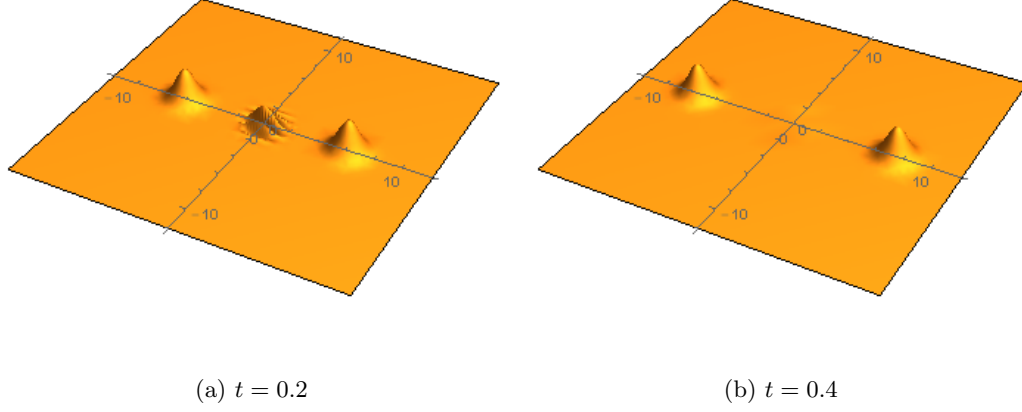


Figure 3.5: $\rho(t, x)$ for cat state initially centred symmetrically on the position axis under the effects of a hyperbolic Hamiltonian and a scattering environment. Note how the interference in the centre rapidly decays while the Gaussian peaks separate.

We see that as before, the interference terms around the origin rapidly decay, and indeed, if we look at the Hilbert-Schmidt norm, we see this clearly as is shown in Fig.3.6.

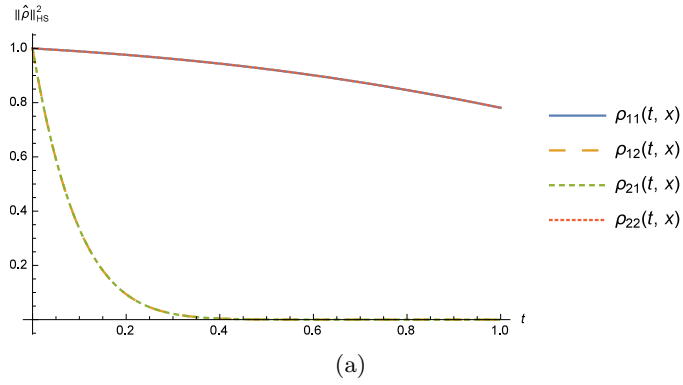
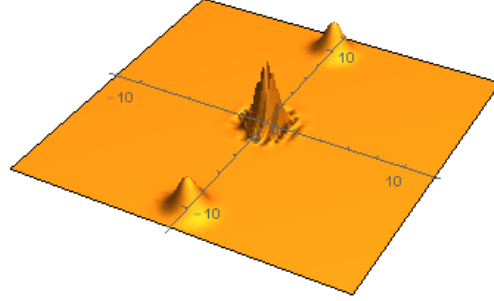


Figure 3.6: The Hilbert-Schmidt norm for each of the individual $\rho_{jk}(t, x)$ in Lemma 3.2.6 for a hyperbolic Hamiltonian and a scattering environment initialised on the q -axis. Note that the cross terms $j \neq k$ decay much more rapidly.

Let us now change our initial cat state to be centred symmetrically along the p axis at

$$y_1 = \begin{pmatrix} 0 \\ 10 \end{pmatrix}, \quad y_2 = \begin{pmatrix} 0 \\ -10 \end{pmatrix}. \quad (3.2.87)$$

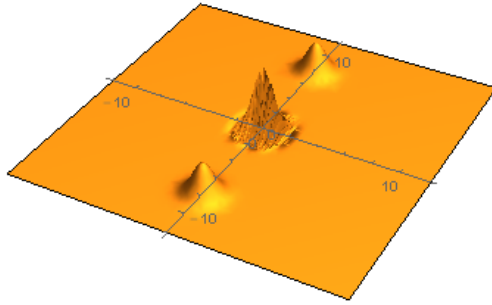
Then the initial state is given in Fig. 3.7



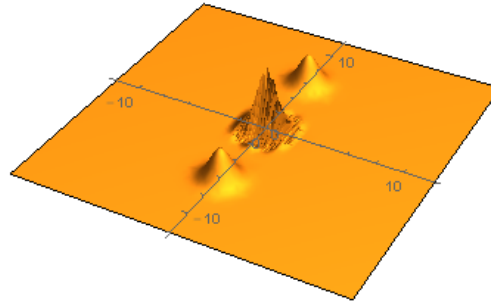
(a) $t = 0$

Figure 3.7: $\rho(0, x)$ for a cat state composed of a superposition of two Gaussian coherent states centred symmetrically on the momentum axis at $p = \pm 10$. Note the highly oscillatory interference terms around the origin.

If we evolve this state using Lemma 3.2.5 we find that the Gaussian peaks move towards each other along the p -axis and, more importantly, the interference terms in the centre *do not* decay, as is shown in Fig. 3.8.



(a) $t = 0.25$



(b) $t = 0.5$

Figure 3.8: $\rho(t, x)$ for cat state initially centred symmetrically on the momentum axis under the effects of a hyperbolic Hamiltonian and a scattering environment. Note how the interference in the centre does not decay as the individual Gaussian states converge.

Indeed if we compare the Hilbert-Schmidt norms again, we find that they all decay at the same rate, as is shown in Fig. 3.9.

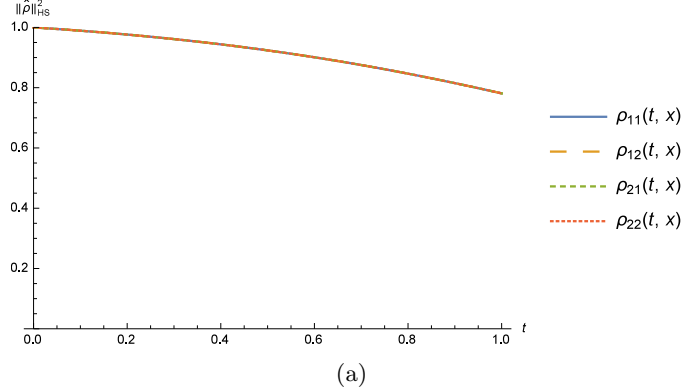


Figure 3.9: The Hilbert-Schmidt norm for each of the individual $\rho_{jk}(t, x)$ in Lemma 3.2.6 for a hyperbolic Hamiltonian and a scattering environment initialised on the p -axis. Note that all terms decay at the same rate.

This suggests that there is a protected subspace that is insulated from effects of decoherence. Perhaps it is no surprise that this subspace seems to be the p axis where $q = 0$ since our Lindblad operator itself is proportional to q .

The above results are all for *Gaussian states*. Now we wish to generalise these results to arbitrary states. To do this we will introduce a projection onto frequencies $|\xi| > s$ where we have taken $s \geq 0$. The projection is defined as follows:

$$(\pi_s \rho)(x) := \frac{1}{(2\pi\hbar)^n} \int_{|\xi| \geq s} e^{\frac{i}{\hbar} x \cdot \xi} \chi_\rho(\xi) d\xi. \quad (3.2.88)$$

This projection is onto the parts of the state which oscillate with a frequency of at least size s/\hbar . The following result shows that this oscillatory part is suppressed rapidly under the Lindblad evolution as long as our matrix D_t is non-degenerate for $t > 0$.

Theorem 3.2.9. *Suppose that $D_t \geq d_t I$ where I is the $2n \times 2n$ identity matrix, and for $t > 0$ we have that $d_t > 0$. Then, for any $\hat{\rho}_0$ in trace class we have that the time evolved state $\hat{\rho}_t$ satisfies for $t > 0$ and $s > 0$*

$$|\pi_s \rho_t(x)| \leq \text{tr} |\hat{\rho}_0| \frac{4}{d_t^n} \Gamma\left(n, \frac{d_t s^2}{2\hbar}\right) \quad (3.2.89)$$

and the Hilbert-Schmidt norm is given by

$$\|\widehat{\pi_s \rho_t}\|_{HS}^2 \leq (\text{tr} |\hat{\rho}_0|)^2 \frac{4}{(2d_t)^n} \Gamma\left(n, \frac{d_t s^2}{2\hbar}\right) \quad (3.2.90)$$

where

$$\Gamma(n, a) := \frac{1}{\Gamma(n)} \int_a^\infty e^{-r} r^{n-1} dr \quad (3.2.91)$$

is a normalised incomplete gamma function.

Proof. Using the theorem 3.2.1 and the definition of π_s we have that

$$|\pi_s \rho_t(x)| \leq \frac{1}{(2\pi\hbar)^n} \int_{|\xi| \geq s} |\chi_0(R_t^T \xi)| e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} d\xi \quad (3.2.92)$$

and using the fact that $|\chi_0(\nu)| \leq \text{tr} |\hat{\rho}_0|$ and for our choice of D_t we have $\xi \cdot D_t \xi \geq d_t |\xi|^2$ we have

$$|\pi_s \rho_t(x)| \leq \frac{\text{tr} |\hat{\rho}_0|}{(2\pi\hbar)^n} \int_{|\xi| \geq s} e^{-\frac{1}{2\hbar} d_t |\xi|^2} d\xi. \quad (3.2.93)$$

Now making the integral substitution $\xi = \sqrt{\frac{2\hbar}{d_t}} \eta$ we obtain the following

$$\int_{|\xi| \geq s} e^{-\frac{1}{2\hbar} d_t |\xi|^2} d\xi = \frac{1}{(d_t \pi)^n} \int_{|\eta|^2 \geq a} e^{-|\eta|^2} d\eta \quad (3.2.94)$$

where $a = \frac{s^2 d_t}{2\hbar}$. This integral can be solved directly by introducing polar coordinates (or looking up standard results) to obtain

$$\int_{|\eta|^2 \geq a} e^{-|\eta|^2} d\eta = 4\pi^n \Gamma(n, a). \quad (3.2.95)$$

Where $\Gamma(n, a)$ is the incomplete gamma function defined in the theorem. Combining everything then we have

$$|\pi_s \rho_t(x)| \leq \text{tr} |\hat{\rho}_0| \frac{4}{d_t^n} \Gamma\left(n, \frac{d_t s^2}{2\hbar}\right) \quad (3.2.96)$$

completing the proof of the first result.

The second result is proved identically but starting from

$$\|\widehat{\pi_s \rho_t}\|_{\text{HS}}^2 \leq \frac{1}{(2\pi\hbar)^n} \int_{|\xi| \geq s} |\chi_0(R_t^T \xi)|^2 e^{-\frac{1}{\hbar} \xi \cdot D_t \xi} d\xi \quad (3.2.97)$$

and proceeding from there. □

Note that the normalised incomplete gamma function $\Gamma(n, a)$ decays extremely rapidly,

$$\Gamma(n, a) \ll e^{-(1-\epsilon)a}, \quad \forall \epsilon > 0 \quad (3.2.98)$$

and hence the highly oscillatory parts of the density operator are quickly damped.

3.3 The Hörmander condition

In this section we will introduce the Hörmander condition [20] which can be thought of as a condition guaranteeing smoothness of solutions to a PDE and some basic background from the theory of PDEs.

Consider a differential operator \mathcal{P} . Broadly Hörmander's condition tells us that for the equation

$$\mathcal{P}u = f, \quad (3.3.1)$$

if f is smooth then u is also smooth.

Here we will broadly follow the background presented in the short review article [47] in order to introduce the Hörmander condition before briefly describing why what on the surface is a condition about smoothness might tell us something about the spread of noise, which is often characterised by large oscillations, in a system. Finally we will relate this condition to some similar results from control theory to assist in this motivation.

We start by considering a general partial differential operator of degree m on \mathbb{R}^n

$$\mathcal{P} = \sum_{|\alpha| \leq m} a_\alpha(x) \partial_x^\alpha \quad (3.3.2)$$

which has smooth coefficients $a_\alpha \in C^\infty(\mathbb{R}^n)$. Now we wish to consider a PDE of the form

$$\mathcal{P}u = f \quad (3.3.3)$$

where we are allowing u and f to be distributions.

If we know f what can we say about u ? It is clear that we can't determine u completely from f since \mathcal{P} can have non-trivial null-spaces but can we determine if certain *properties* of f are inherited by u ? In particular, if we suppose that f is smooth, is u smooth? Under what conditions is this smoothness inherited?

We call an operator \mathcal{P} that allows smoothness to be inherited in this way to be *hypoelliptic*, or more precisely:

Definition 3.3.1. A differential operator \mathcal{P} is called *hypoelliptic* at $x_0 \in \mathbb{R}^n$ if whenever $\mathcal{P}u \in C^\infty$ on a neighbourhood of x_0 then $u \in C^\infty$ in that neighbourhood too.

For example, on \mathbb{R} if we take $\mathcal{P} = \frac{d}{dx}$ then \mathcal{P} is hypoelliptic at every point $x_0 \in \mathbb{R}$ since by the fundamental theorem of calculus we can determine $u(x)$ directly as

$$u(x) = \int_{x_0}^x \mathcal{P}u(x') dx' + C. \quad (3.3.4)$$

On the other hand, $\mathcal{P} = \frac{\partial}{\partial x_1}$ in \mathbb{R}^n is *not* hypoelliptic since *any* choice of $u = u(x_2, x_3, \dots, x_n)$ even a completely non-smooth u will return $\mathcal{P}u = 0$.

If we want to make this definition more quantitative we can introduce some results from the theory of Sobolev spaces. Let $p \in [1, \infty]$ and $s \in \mathbb{R}$. We denote the L^p Sobolev space of order s on \mathbb{R}^n by L_s^p (in contrast to the usual $W^{s,p}$ notation). If s is an integer then this is just the Banach space of distributions ν such that $\partial^\alpha \nu \in L^p$, $|\alpha| \leq s$.

Also, for two functions $\phi_1, \phi_2 \in C_0^\infty(\mathbb{R}^n)$ we say that $\phi_1 \prec \phi_2$ if $\phi_2 \equiv 1$ on a neighbourhood of the support of ϕ_1 . Similarly, we write that $\{x_0\} \prec \phi_1$ if $\phi_1 \equiv 1$ in a neighbourhood of $\{x_0\}$.

The famous Sobolev embedding theorem has as a consequence that $\nu \in C^\infty$ near $x_0 \in \mathbb{R}^n$ if and only if there exists a function $\{x_0\} \prec \phi_1 \in C_0^\infty$ such that $\phi \nu \in \cap_s L_s^2$. This directly leads to the following lemma:

Lemma 3.3.2. *Let $\{x_0\} \prec \phi_1 \prec \phi_2$. Suppose that for all $s \in \mathbb{R}$ there exists a $r(s) \in \mathbb{R}$ such that*

$$\phi_2 \mathcal{P}u \in L_{r(s)}^2 \implies \phi_1 u \in L_s^2. \quad (3.3.5)$$

Then \mathcal{P} is hypoelliptic at x_0 .

The Laplacian on \mathbb{R}^n is one of the classic examples of a hypoelliptic operator and in fact is the most common example of an even more restricted class, the *elliptic* operators.

Definition 3.3.3. We say that a partial differential operator \mathcal{P} is *elliptic* at x_0 if the sum

$$\sum_{|\alpha|=m} a_\alpha(x_0) \xi^\alpha = 0 \quad (3.3.6)$$

only if $\xi = 0$.

One can show that all elliptic operators are also hypoelliptic but importantly the reverse is *not* true. When looking for the operators that are hypoelliptic but not elliptic things become a bit more subtle. We now introduce a less restrictive form of ellipticity as follows:

Definition 3.3.4. \mathcal{P} is *subelliptic* at x_0 if there exists an $\epsilon > 0$ such that the conditions of Lemma 3.3.2 hold with $r(s) = s - \epsilon$.

This tells us that if \mathcal{P} is subelliptic at x_0 , then u is smoother than $\mathcal{P}u$ by ϵ derivatives in L^2 Sobolev space. Ellipticity is the same condition but with the restriction that $\epsilon = m$. Hence subellipticity can be much weaker than ellipticity but it maintains the property that all subelliptic operators are hypoelliptic. Identifying operators that are subelliptic is much harder than identifying elliptic operators.

We now give the general form of the Hörmander condition which we will later specialise.

Definition 3.3.5. Suppose we have a set of vector fields X_j for $j = 0, 1, \dots, K$ on \mathbb{R}^n and consider the subspaces $V_k \subset \mathbb{R}^n$, $k = 0, 1, 2, \dots$ spanned by the vector fields X_j and their iterated commutators

$$V_0(x) := \text{span}\{X_0(x), X_1(x), \dots, X_K(x)\} \quad (3.3.7)$$

$$V_k(x) := \text{span}\{Y(x), [Y, X_j](x) \mid Y \in V_{k-1}(x), j = 0, 1, 2, \dots, K\}. \quad (3.3.8)$$

We say that $X_j, j = 0, 1, \dots, K$ satisfy the *Hörmander condition* if for some k we have $V_k(x) = \mathbb{R}^n$ for all $x \in \mathbb{R}^n$. If the Hörmander condition holds then we call the smallest integer k_x such that $V_{k_x}(x) = \mathbb{R}^d$ the local rank at x and $k = \sup_x k_x$ the global rank.

Now define

$$\mathcal{L} = \sum_0^K X_j^* X_j + X_0 \quad (3.3.9)$$

where X_j^* denotes the L^2 adjoint. One can think of this as a generalisation of the Laplacian known as the *Hörmander sub-Laplacian* (if $X_j = \frac{\partial}{\partial x_j}$ then $\mathcal{L} = \Delta$). Hörmander proved that if the vector fields X_j satisfy this condition at x_0 then \mathcal{L} is subelliptic (and hence hypoelliptic) at x_0 [20].

This condition in sub-Riemannian geometry and control theory is also known as the Chow condition or the bracket condition. To give some insight into its meaning let's denote by ϕ_k^t the flow generated by the vector field X_k . Then we have that

$$\phi_k^{-t} \circ \phi_{k'}^{-t} \circ \phi_k^t \circ \phi_{k'}^t = t^2 [X_k, X_{k'}] + O(t^3). \quad (3.3.10)$$

By combining the flows of the vector fields X_k we can move in a direction given by a commutator $[X_k, X_{k'}]$. If we iterate this argument we can show that suitable compositions of flows allow us to move in the direction of iterated commutators as well.

In linear control theory the main focus of study is linear differential equations of the following form

$$\dot{x} = \sum_{k=0}^K u_k(t) X_k(x) \quad (3.3.11)$$

where in this case the $X_k, k = 0, \dots, K$ are given vector fields and the functions $u_k(t) \in L^1([0, T]), k = 0, \dots, K$ are the control inputs which are to be chosen. If there exists a set of control inputs $u_k(t)$ such that the solution $x(t)$ to (3.3.11) with initial condition $x(0) = x_0$ satisfies $x(T) = x_1$ then we say a point $x_1 \in \mathbb{R}^n$ can be reached from x_0 . If any two points $x_0, x_1 \in \mathbb{R}^n$ can be reached from one another with a suitable set of control inputs $u_k(t)$ then we say the system is *controllable*.

Theorem 3.3.6 (Chow Rashevsky Theorem [4]). *Assume that the vector fields $X_k, k = 0, \dots, K$ on a connected manifold M satisfy Hörmander's condition. Then the system 3.3.11 is controllable.*

If we now compare this with the form of the Lindblad equation on phase space (2.6.14) we see that we can readily identify the vector fields X_i . The rationale for considering this condition then becomes more apparent, we had vector fields X_0 which corresponded to a transport and then a set of vector fields X_j which described a diffusion. By considering the Hörmander condition we are asking whether the combination of the transport from X_0 and the diffusion provides enough mixing to reach all degrees of freedom in the system. This can then be related to the spread of decoherence in the system.

3.4 Decoherence and Hörmander

We start by adapting the definition we gave at the end of the background chapter (2.8.2) to the context of the Lindblad systems we have been studying.

Definition 3.4.1. For a system defined by the Lindblad equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}[\hat{\mathcal{H}}, \hat{\rho}] + \frac{1}{2\hbar} \sum_j [\hat{L}_j \hat{\rho}, \hat{L}_j^\dagger] - [\hat{\rho} \hat{L}_j^\dagger, \hat{L}_j]. \quad (3.4.1)$$

we say that it shows **decoherence in phase space** if for any $\hat{\rho}_0 \in \mathcal{T}$ the symbol $\rho_t(x)$ of the time evolved operator $\hat{\rho}_t$ is in $S_{\frac{1}{2}}^0$ for $t \geq T > 0$ uniformly. That is, for any $T > 0$ and any multi-index α there exists a constant $C_{T,\alpha} > 0$ such that

$$\sup_{\substack{x \in \mathbb{R}^n \\ t \geq T}} |\partial_x^\alpha \rho_t(x)| \leq C_{T,\alpha} \hbar^{-|\alpha|/2}. \quad (3.4.2)$$

for all $\hbar \in (0, 1]$.

Now lets try and relate this definition to the Hörmander condition. Recall we had the following form of the Lindblad equation (see (2.6.14)) written in terms of the vector fields X_0, \dots, X_{2K} :

$$\partial_t \rho = X_0 \rho + \nabla \cdot X_0 \rho + \frac{\hbar}{2} \sum_{k=1}^{2K} X_k^2 \rho. \quad (3.4.3)$$

where

$$X_0 \rho = \{H, \rho\} + \sum_k \text{Im } L_k \{ \text{Re } L_k, \rho \} - \text{Re } L_k \{ \text{Im } L_k, \rho \}, \quad (3.4.4)$$

with

$$\nabla \cdot X_0 = 2 \sum_k \{ \text{Re } L_k, \text{Im } L_k \} \quad (3.4.5)$$

and

$$X_k \rho = \{ \text{Re } L_k, \rho \}, \quad X_{K+k} \rho = \{ \text{Im } L_k, \rho \} \quad (3.4.6)$$

for $k = 1, \dots, K$.

We would like to evaluate the Hörmander condition for this set of vector fields under the restrictions that H is quadratic and the L_k 's are linear, parametrising as before $L_k = x \cdot \Omega l_k$ and $H = \frac{1}{2} x \cdot H'' x$. Note that the point $x = 0$ is special in that $X_0(0) = 0$. Hence $V_k(0)$ is necessarily smaller than $V_k(x)$ for $x \neq 0$ and hence is the most important case. In what follows we always assume we consider $x = 0$. Then we can reduce the Hörmander condition 3.3.5 to the following form:

Lemma 3.4.2. *Define*

$$V_0 = \text{span}\{ \text{Re } l_k, \text{Im } l_k \mid k = 1, \dots, K \} \subset \mathbb{R}^{2n} \quad (3.4.7)$$

and

$$V_k = V_0 + FV_0 + F^2V_0 + \cdots + F^kV_0 \subset \mathbb{R}^{2n} \quad (3.4.8)$$

for $k = 1, 2, \dots$. Then the vector fields X_0, X_1, \dots, X_{2K} satisfy Hörmander's condition for all $x \in \mathbb{R}^{2n}$ if and only if there is an $r \leq 2n - 1$ such that $V_r = \mathbb{R}^{2n}$.

Proof. We know that constant vector fields commute, hence we only have to consider the commutators $[X_0, X_j]$ and directly computing these we get

$$[X_0, X_k]\rho = (A \operatorname{Re} l_k) \cdot \nabla \rho \quad (3.4.9)$$

and

$$[X_0, X_{k+K}]\rho = (A \operatorname{Im} l_k) \cdot \nabla \rho. \quad (3.4.10)$$

Clearly these are also constant vector fields and thus commute with each other and all of the X_j vector fields. This reduces our problem to considering only j -fold commutators of X_0 with a single X_k for $k = 1, \dots, K$. Computing these we get

$$[X_0, [X_0, [\cdots, X_k] \cdots]] = A^j \operatorname{Re} l_k \quad (3.4.11)$$

and

$$[X_0, [X_0, [\cdots, X_{k+K}] \cdots]] = A^j \operatorname{Im} l_k. \quad (3.4.12)$$

Now we know that $X_0(x)$ vanishes at $x = 0$ and because of this it does not contribute to $V_0 = V_0(0)$ and hence we find $V_1 = V_0 + AV_0$, $V_2 = V_0 + AV_0 + A^2V_0$ and so on. However, we know that the image of N is contained in V_0 and hence $AV_0 \subset V_0 + FV_0$ which gives us that $V_1 = V_0 + FV_0$. We can repeat this argument to get that $V_k = V_0 + FV_0 + \cdots + F^kV_0$.

Hörmander's condition now reduces to showing that $V_k = \mathbb{R}^{2n}$ for some k . By the Cayley-Hamilton theorem we know that F^{2n+r} for $R \geq 0$ can be expressed as a polynomial in F of order $2n - 1$, hence we know that $V_k = V_{2n-1}$ for all $k \geq 2n$. \square

Example 3.4.3 (Example systems).

- (i) An obvious choice for a system which will always satisfy the Hörmander condition as described above is one where we describe the environment by a set of $2n$ linearly independent Lindblad operators (in the sense that the l_j 's are linearly independent or that for n of the Lindblad operators the real and imaginary parts are linearly independent). In this case

$$V_0 = \operatorname{span}\{\operatorname{Re} l_k, \operatorname{Im} l_k | k = 1, \dots, 2n\} = \mathbb{R}^{2n} \quad (3.4.13)$$

immediately and no further calculation is required.

- (ii) Let's consider again a one dimensional system, $x = (q, p) \in \mathbb{R}^2$ described by a harmonic oscillator Hamiltonian with symbol

$$H(x) = \frac{1}{2}x \cdot H''x, \quad H'' = \begin{pmatrix} \omega & 0 \\ 0 & \omega \end{pmatrix}, \quad \omega \in \mathbb{R} \quad (3.4.14)$$

interacting with a point scatterer environment described by a single Lindblad operator with symbol

$$L(x) = \sqrt{\sigma}q, \quad \sigma \in \mathbb{R}. \quad (3.4.15)$$

Writing this symbol as

$$L(x) = \Omega l \cdot x, \quad l = \begin{pmatrix} 0 \\ \sqrt{\sigma} \end{pmatrix} \quad (3.4.16)$$

we see immediately that

$$V_0 = \text{span}\{\text{Re } l, \text{Im } l\} = \text{span}\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\} \cong \mathbb{R}. \quad (3.4.17)$$

Clearly as $V_0 \not\cong \mathbb{R}^2$ we haven't satisfied Hörmander's condition yet, and we need to go further. Consider now V_1 , we had that

$$V_1 = V_0 + FV_0 \quad (3.4.18)$$

where we can calculate $F = \Omega H'' = \begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix}$.

Using this we have

$$FV_0 = \text{span}\left\{\begin{pmatrix} 0 & \omega \\ -\omega & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\} = \text{span}\left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right\}. \quad (3.4.19)$$

Clearly then

$$V_1 = \text{span}\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right\} \cong \mathbb{R}^2 \quad (3.4.20)$$

and Hörmander's condition is satisfied. Note that this corresponds to Example 3.2.7 where we saw decoherence occurred independent of the choice of the starting position of the cat state, although as mentioned the *rate* of decoherence *was* dependent on this initial position.

- (iii) Let's take the exact same example but instead of a harmonic oscillator Hamiltonian we have a hyperbolic Hamiltonian

$$H'' = \begin{pmatrix} 0 & \gamma \\ \gamma & 0 \end{pmatrix}, \quad \gamma \in \mathbb{R}. \quad (3.4.21)$$

In this case V_0 is clearly unchanged, but

$$FV_0 = \text{span}\left\{\begin{pmatrix} \gamma & 0 \\ 0 & -\gamma \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\} = \text{span}\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\} \quad (3.4.22)$$

and hence

$$V_1 = \text{span}\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\} \cong \mathbb{R} \neq \mathbb{R}^2. \quad (3.4.23)$$

Thus the Hörmander condition is not satisfied. This corresponds to Example 3.2.8 where we saw that there was a particular subspace defined by $q = 0$ along which there was no onset of decoherence at all. If we compare this to the result above, we see that we have decoherence reaching the subspace defined by

$$\text{span} \left\{ \Omega \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\} = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right\} \quad (3.4.24)$$

but the subspace defined by $\text{span} \left\{ \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$ is never reached.

- (iv) Finally, let us consider a more complicated system. Suppose we have two one dimensional harmonic oscillators with frequencies ω_1 and ω_2 respectively, and suppose we consider a nearest neighbour Hooke-like coupling model with an interaction parameter δ , see for instance [39][19][26], then in terms of the symbols of creation and annihilation operators we have the symbol Hamiltonian

$$H(x) = \frac{\omega}{2} \sum_{j=1}^2 a_j^\dagger a_j + \delta \left(a_j^\dagger a_{j+1} + a_{j+1}^\dagger a_j \right) \quad (3.4.25)$$

which describes energy level jumps between systems. In terms of the standard coordinates q_i and p_i we have

$$H(x) = \frac{1}{2} \sum_{j=1}^2 \omega (q_j^2 + p_j^2) + \delta (q_1 q_2 + p_1 p_2). \quad (3.4.26)$$

for $x = (q_1, p_1, q_2, p_2)$, If we write

$$H(x) = \frac{1}{2} x \cdot H'' x \quad (3.4.27)$$

then

$$H'' = \begin{pmatrix} \omega_1 & 0 & \delta & 0 \\ 0 & \omega_1 & 0 & \delta \\ \delta & 0 & \omega_2 & 0 \\ 0 & \delta & 0 & \omega_2 \end{pmatrix}. \quad (3.4.28)$$

As before we take a scattering environment but we only couple it to the first oscillator. That is

$$L(x) = \sqrt{\sigma} q_1 = \Omega_2 l \cdot x \quad \text{for } \Omega_2 = \begin{pmatrix} \Omega & 0 \\ 0 & \Omega \end{pmatrix}, l = \begin{pmatrix} 0 \\ \sqrt{\sigma} \\ 0 \\ 0 \end{pmatrix}. \quad (3.4.29)$$

In this case,

$$V_0 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\} \cong \mathbb{R}. \quad (3.4.30)$$

Continuing,

$$FV_0 = \text{span} \left\{ F \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\} = \text{span} \left\{ \begin{pmatrix} \omega_1 \\ 0 \\ \delta \\ 0 \end{pmatrix} \right\} \quad (3.4.31)$$

where we have used that $F = \Omega_2 H''$. This is clearly linearly independent and hence

$$V_1 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_1 \\ 0 \\ \delta \\ 0 \end{pmatrix} \right\} \cong \mathbb{R}^2. \quad (3.4.32)$$

If we continue in this fashion, computing FV_1 , we find that

$$V_2 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_1 \\ 0 \\ \delta \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \delta^2 + \omega_1^2 \\ 0 \\ \delta(\omega_1 + \omega_2) \end{pmatrix} \right\} \quad (3.4.33)$$

and finally, computing FV_2 ,

$$V_3 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_1 \\ 0 \\ \delta \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \delta^2 + \omega_1^2 \\ 0 \\ \delta(\omega_1 + \omega_2) \end{pmatrix}, \begin{pmatrix} \omega_1^3 + \delta^2(\omega_2 + 2\omega_1) \\ 0 \\ \delta^3 + \delta(\omega_1^2 + \omega_1\omega_2 + \omega_2^2) \\ 0 \end{pmatrix} \right\}. \quad (3.4.34)$$

It is not clear immediately whether these four vectors are linearly independent, and thus it is not clear whether $V_3 \cong \mathbb{R}^4$. If we compute the determinant of the matrix, which we call E , whose column vectors are given by these 4 vectors, we find that

$$\det E = \delta^2(\omega_1 + \omega_2)^2(\omega_1\omega_2 - \delta^2). \quad (3.4.35)$$

The Hörmander condition fails when $\det E = 0$. Clearly this occurs when $\delta = 0$ as we would expect, since this corresponds to the two harmonic oscillators not interacting at all, and hence there is no path for the effect of the environment to reach the second oscillator.

It also occurs when $\omega_1 = -\omega_2$ so that the oscillators have opposite frequency. This is somewhat nonphysical since we usually assume that the frequency is positive. If we look at the calculation of V_2 , we see that, in this situation, this means that the third vector becomes just the span of a multiple of e_2 (the standard basis vector) and hence provides access to no new space in the system.

Finally there is another case when the Hörmander condition fails, namely when

$$\delta^2 = \omega_1\omega_2. \quad (3.4.36)$$

In this case H is no longer positive definite and as a result there is no ground state. This then represents a possibly non-physical situation that is not explicitly discounted.

While the vector spaces V_k defined in (3.4.2) are very directly obtainable, as the examples (3.4.3) illustrate, they aren't particularly suited to understanding the spread of decoherence throughout the system. In the second example we can see directly that the effect of the environment, and hence decoherence, spreads first to the subspace spanned by the basis vector e_2 , and then to the subspace spanned by e_1 . In example (iv) however it is much more difficult to characterise which subspaces of our system are being affected and indeed these subspaces depend intimately on the choice of parameters in our system.

Towards this end we will introduce a new partition of phase space into orthogonal subspaces which is adapted to the commutators of the vectorfields X_k , $k = 0, 1, \dots, 2K$. We start by defining

$$W_0 := V_0 \quad (3.4.37)$$

and take W_k to be the orthogonal complement of V_{k-1} in V_k . Then we have the following:

$$V_k = W_0 \oplus W_1 \oplus \dots \oplus W_k \quad \text{and for } k \neq j \quad W_k \perp W_j. \quad (3.4.38)$$

Now, if the Hörmander condition *doesn't* hold then there is a smallest r such that $V_{r+1} = V_r$ and $V_r \neq \mathbb{R}^{2n}$. We define W_{df} to be the orthogonal complement of V_r in \mathbb{R}^{2n} . Hence we can write

$$\mathbb{R}^{2n} = W_0 \oplus W_1 \oplus \dots \oplus W_r \oplus W_{df}. \quad (3.4.39)$$

Here we use the notation W_{df} to indicate that W_{df} is, as we will see, the *decoherence free* subspace of our system. If we take $W_{df} = \{0\}$ then formally the Hörmander condition holds and we can include it in our framework.

Example 3.4.4 (Orthogonal decomposition for a chain of 2 Harmonic oscillators).

Let's return to example 3.4.3 (iv) to illustrate this. We start by taking W_0 equal to V_0 , given by (3.4.30), to get

$$W_0 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\}. \quad (3.4.40)$$

We now consider the orthogonal complement of $V_0 = W_0$ in the space V_1 , given by (3.4.32), which it gives immediately as

$$W_1 = \text{span} \left\{ \begin{pmatrix} \omega_1 \\ 0 \\ \delta \\ 0 \end{pmatrix} \right\}. \quad (3.4.41)$$

We now continue and consider the orthogonal complement of $V_1 = W_0 \oplus W_1$ in the space V_2 , given by (3.4.33). If $\delta \neq 0$ and $\omega_1 \neq \omega_2$, we see that this is just

$$W_2 = \text{span} \left\{ \begin{pmatrix} 0 \\ 0 \\ 0 \\ \delta(\omega_1 + \omega_2) \end{pmatrix} \right\}. \quad (3.4.42)$$

Finally, if we consider the orthogonal complement of $V_2 = W_0 \oplus W_1 \oplus W_2$ in V_3 given by (3.4.34) we find the result

$$W_3 = \text{span} \left\{ \begin{pmatrix} \delta^2(\omega_1 + \omega_2)(\delta^2 - \omega_1\omega_2) \\ 0 \\ \delta\omega_1(\omega_1 + \omega_2)(\omega_1\omega_2 - \delta^2) \\ 0 \end{pmatrix} \right\}. \quad (3.4.43)$$

We see then, as described before, if $\delta = 0$ then Hörmander's condition is not satisfied and in particular W_2 and W_3 are just the trivial subspaces containing the origin. This corresponds to no interaction and no effect of decoherence travelling between the two oscillators so that the effect of the scattering environment is isolated entirely on the first oscillator. In this case

$$W_{df} = \text{span} \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\}. \quad (3.4.44)$$

In the case where $\omega_1 = -\omega_2$ then W_2 and W_3 are also simply the trivial subspaces, however in this case the decoherence free subspace is less simple to interpret since it is not isolated to one oscillator. In this case

$$W_{df} = \text{span} \left\{ \begin{pmatrix} \delta \\ 0 \\ -\omega_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \right\}. \quad (3.4.45)$$

Finally, our last case when $\delta^2 = \omega_1\omega_2$. In this situation only W_3 is trivial, and we only have a one dimensional decoherence free subspace given by

$$W_{df} = \text{span} \left\{ \begin{pmatrix} \delta \\ 0 \\ -\omega_1 \\ 0 \end{pmatrix} \right\}. \quad (3.4.46)$$

We saw before in Example 3.2.8 that if our initial cat state was centred on what we now would call W_0 , or more correctly ΩW_0 , then we see the HS norm of the cross terms $\|\rho_{12}(t, x)\|_{HS}^2$ decays rapidly, indicating the onset of decoherence. However, if we are in

the decoherence free subspace, then these terms do not experience rapid decay due to decoherence.

Let's consider this final case, where $\delta^2 = \omega_1 \omega_2$ and let's compute $\|\rho_{12}(t, x)\|_{HS}^2$ for 4 cat states initial centred on the subspaces W_0 , W_1 , W_2 and W_3 respectively such that the cartesian distance between the two centres is the same. From the calculations above, we expect W_3 to be the decoherence free subspace, and indeed we see this in Fig. 3.10.

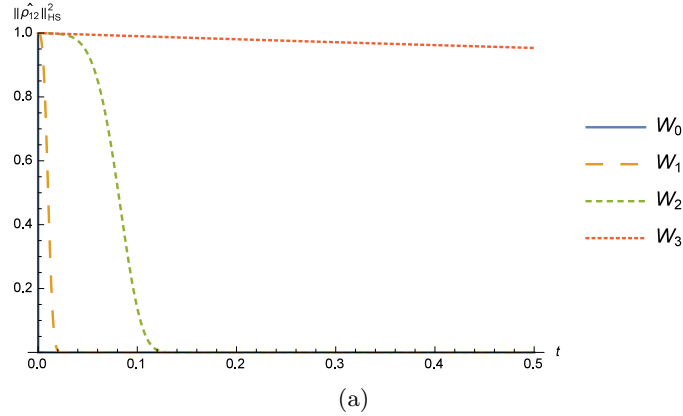


Figure 3.10: The Hilbert-Schmidt norm of $\rho_{12}(t, x)$ in Lemma 3.2.6 for a chain of two Harmonic oscillators and a scattering environment initialised in the subspaces W_i , $i = 0, \dots, 3$ for $\hbar = 10^{-5}$, $\omega_1 = \omega_2 = \delta = 1$ and $\sigma = 0.1$. Note that timelag in the onset of the decay and that the state initialised in W_3 does not experience decoherence.

If we now change $\delta = \frac{1}{2}$ then the subspace W_3 does experience decoherence as is shown in Fig. 3.11.

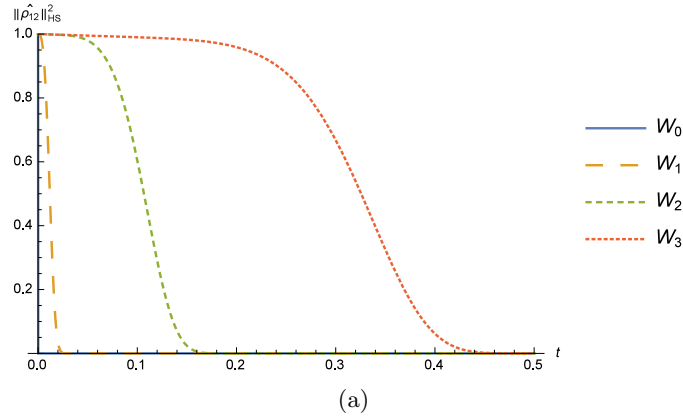


Figure 3.11: The Hilbert-Schmidt norm of $\rho_{12}(t, x)$ in Lemma 3.2.6 for a chain of two Harmonic oscillators and a scattering environment initialised in the subspaces W_i , $i = 0, \dots, 3$ for $\hbar = 10^{-5}$, $\omega_1 = \omega_2 = \delta = \frac{1}{2}$ and $\sigma = 0.1$. Note that timelag in the onset of the decay.

We now wish to investigate the timescales on which decoherence spreads through the system. We utilise the ideas of Lanconelli and Polidoro [32] in the field of sub-Riemannian geometry where they introduce the idea of “nilpotentization”. By using this, we reduce our system to a simpler system which has the same short time evolution and in particular for our purposes, the same structure when it comes to the separation of timescales.

To this end we consider the orthogonal projections onto the subspaces W_j which we denote by P_j . Note that

$$P_j l_k = \delta_{j,0} l_k \quad (3.4.47)$$

for $k = 1, \dots, K$ and we have the usual resolution of identity result

$$I = P_0 + P_1 + \dots + P_{r+1}. \quad (3.4.48)$$

Ultimately we wish to investigate the timescales of D_t and C_t , which themselves depend on the object $R_t = e^{tA}$. Hence we investigate A and powers of A projected onto the subspaces W_i .

Lemma 3.4.5. *Let $i \geq j + 2$. then we have*

$$P_i A P_j = 0 \quad (3.4.49)$$

and for $i \geq 1$ we have

$$P_i A P_j = P_i F P_j. \quad (3.4.50)$$

Also, for $i > j + k + 1$ we have

$$P_i A^k P_j = 0 \quad (3.4.51)$$

and finally for $i = j + k$ we have

$$P_i A^k P_j = P_i F P_{i-1} F P_{i-2} F \dots P_{j+1} F P_j. \quad (3.4.52)$$

Proof. First recall the form of A :

$$A = F + N\Omega \quad (3.4.53)$$

and note that the image of N is in W_0 . Thus $P_i N = 0$ for any $i \geq 1$. Clearly then

$$P_i A P_j = P_i F P_j. \quad (3.4.54)$$

Because $A : V_j \rightarrow V_{j+1}$ and $V_{j+1} = V_j \oplus W_{j+1}$ with $W_j \subset V_j$ and $W_{j+1} \subset V_{j+1}$, we have

$$P_i A P_j = 0 \quad (3.4.55)$$

if $i \geq j + 2$, completing the proof of the first two results.

For the next two results involving powers of A lets first consider the simplest case where $k = 2$ which will instruct how the general result will be proved. Using the resolution of identity result we can write

$$P_i A^2 P_j = \sum_{i_1} P_i A P_{i_1} A P_j. \quad (3.4.56)$$

We consider some separate cases. First, if $i \geq j + 3$ then for each term in this sum we either have

$$i \geq i_1 + 2 \implies P_i A P_{i_1} = 0, \quad (3.4.57)$$

or we have

$$i_1 \geq j + 2 \implies P_{i_1} A P_j = 0 \quad (3.4.58)$$

where we have simply used the result we just proved (3.4.49). Thus for all cases the sum is zero and hence $P_i A^2 P_j = 0$. Now consider the case $i = j + 2$. Then for $i_1 \neq j + 1 = i - 1$ the terms are zero. The only remaining terms are thus, by (3.4.50)

$$P_i A^2 P_j = P_i A P_{j+1} A P_j = P_i F P_{j+1} F P_j. \quad (3.4.59)$$

We can see that these fit the general results we claimed in lemma for $k = 2$ and the proof of the result for general k follows the same idea. We use resolution of identity to write

$$P_i A^k P_j = \sum_{i_1, i_2, \dots, i_{k-1}} P_i A P_{i_{k-1}} A \cdots P_{i_2} A P_{i_1} A P_j \quad (3.4.60)$$

and note that each term in this multi-sum is zero if any consecutive indices increase by at least 2.

Note that if $i - j \geq k + 1$ then this has to happen at least once for each term and thus all terms are zero. If instead $i = j - k$ then there is exactly one non-zero term in the sum, which is the case where each index increases by one at each step. In this case we apply the first results to get

$$P_i A^k P_j = P_i A P_{i-1} A P_{i-2} \cdots A P_j = P_i F P_{i-1} F P_{i-2} \cdots F P_j \quad (3.4.61)$$

completing the proof. \square

This lemma isn't particularly easy to understand in this abstract sense but it can be visualised in matrix form very easily. We write $A_{ij} = P_i A P_j$ and equivalently $F_{ij} = P_i F P_j$. Then the matrix form (A_{ij}) is given by

$$(A_{ij}) = \begin{pmatrix} A_{00} & A_{01} & A_{02} & \cdots & \\ F_{10} & F_{11} & F_{12} & & \\ 0 & F_{21} & F_{22} & & \\ \vdots & & \ddots & & \\ 0 & 0 & 0 & F_{r+1,r} & F_{r+1,r+1} \end{pmatrix} \quad (3.4.62)$$

By writing it in this form we can better understand the leading order behaviour of $R_t P_0 = e^{tA} P_0$. As a result we will introduce a simpler evolution which we will denote by

$$R_t^\sharp = e^{tF^\sharp} \quad (3.4.63)$$

which serves to approximate the small t evolution of $R_t P_0$. To do this we introduce

$$F^\sharp := P_1 F P_0 + P_2 F P_1 + P_3 F P_2 + \cdots \quad (3.4.64)$$

which in matrix form is simply the bottom left off-diagonal of (A_{ij})

$$(F_{i,j}^\sharp) = \begin{pmatrix} 0 & 0 & 0 & \cdots \\ F_{10} & 0 & 0 & \\ 0 & F_{21} & 0 & \\ \vdots & & \ddots & \\ 0 & 0 & 0 & F_{r+1,r} & 0 \end{pmatrix}. \quad (3.4.65)$$

Using this we have the following lemma:

Lemma 3.4.6. *For $i = 0, \dots, r$*

$$P_i R_t P_0 = P_i e^{tA} P_0 = P_i e^{tF^\sharp} P_0 + O(t^{i+1}) \quad (3.4.66)$$

where

$$P_i e^{tF^\sharp} P_0 = \frac{t^i}{i!} P_i F^i P_0. \quad (3.4.67)$$

Proof. This proof is a pretty simple application of the previous lemma. If we expand the exponential we have

$$P_i e^{tA} P_0 = \sum_{\alpha=0}^i \frac{t^\alpha}{\alpha!} P_i A^\alpha P_0 + O(t^{i+1}) \quad (3.4.68)$$

and applying the previous lemma we have that $P_i A^\alpha P_0 = 0$ if $\alpha > i$ and $P_i A^i P_0 = P_i F^i P_0$ and as a result

$$P_i e^{tA} P_0 = \frac{t^i}{i!} P_i F^i P_0 + O(t^{i+1}). \quad (3.4.69)$$

Note that

$$P_i F^{\sharp i} P_0 = P_i F P_{i-1} F \cdots P_1 F P_0. \quad (3.4.70)$$

We introduced (F_{ij}^\sharp) in matrix form since we can easily take powers to visualise this. For example

$$(F_{ij}^\sharp)^2 = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & & \\ F_{21}F_{10} & 0 & 0 & & \\ 0 & F_{32}F_{21} & 0 & & \vdots \\ \vdots & \vdots & \ddots & & \\ 0 & 0 & 0 & F_{r,r-1}F_{r-1,r-2} & 0 & 0 \end{pmatrix}. \quad (3.4.71)$$

Hence we see that

$$F^{\sharp 2} P_0 = F_{21}F_{10} = P_2 F P_1 F P_0 \quad (3.4.72)$$

as expected. Using this we can expand $R_t^\sharp P_0$ to get

$$R_t^\sharp P_0 = e^{tF^\sharp} P_0 = \sum_{k=0}^r \frac{t^k}{k!} F^{\sharp k} P_0 = \sum_{k=0}^r \frac{t^k}{k!} P_k F P_{k-1} F \cdots P_1 F P_0. \quad (3.4.73)$$

and as a result

$$P_i e^{tF^\sharp} P_0 = \frac{t^i}{i!} P_i F P_{i-1} F \cdots P_1 F P_0 = \frac{t^i}{i!} P_i F^i P^0 \quad (3.4.74)$$

completing the proof. \square

Note now that if we recall that $M = \operatorname{Re} \sum_k \bar{l}_k l_k^\top$ and the form of D_t (3.2.5) we can write $D_t(\xi) = \xi \cdot D_t \xi$ as the expansion

$$D_t(\xi) = \sum_{k=1}^K \int_0^t |\xi \cdot R_s l_k|^2 ds. \quad (3.4.75)$$

Equivalently for $C_t(\xi) = \xi \cdot C_t \xi$ we have

$$C_t(\xi) = \sum_{k=1}^K \int_0^t |\xi \cdot R_{-s} l_k|^2 ds. \quad (3.4.76)$$

Plugging in our short time approximation of $R_t = e^{tA}$ which we defined above as $R_t^\sharp = e^{tF^\sharp}$ we get

$$D_t^\sharp(\xi) = \sum_{k=1}^K \int_0^t |\xi \cdot R_s^\sharp l_k|^2 ds, \quad (3.4.77)$$

$$C_t^\sharp(\xi) = \sum_{k=1}^K \int_0^t |\xi \cdot R_{-s}^\sharp l_k|^2 ds. \quad (3.4.78)$$

which allows us to formulate one of the main theorems of this section.

Theorem 3.4.7. *We have the following*

$$D_t(\xi) = D_t^\sharp(\xi)(1 + O(t)) \quad (3.4.79)$$

$$C_t(\xi) = C_t^\sharp(\xi)(1 + O(t)) \quad (3.4.80)$$

$$C_t(\xi) = D_t(\xi)(1 + O(t)) \quad (3.4.81)$$

and for $\xi \in V_{i-1}^\perp = W_i \oplus W_{i+1} \oplus \cdots \oplus W_{r+1}$ we have

$$D_t(\xi) = \frac{1}{(2i+1)(i!)^2} \sum_{k=1}^K |\xi \cdot F^i l_k|^2 t^{2i+1} + O(t^{2i+2}) \quad (3.4.82)$$

which guarantees positivity for small t .

Proof. Since $R_t = R_t^\sharp(1 + O(t))$ we have immediately that

$$D_t(\xi) = D_t^\sharp(\xi)(1 + O(t)) \quad (3.4.83)$$

$$C_t(\xi) = C_t^\sharp(\xi)(1 + O(t)). \quad (3.4.84)$$

$$(3.4.85)$$

By the previous lemma and the fact that $P_0 l_k = l_k$ we have that for $\xi \in W_j \oplus W_{j+1} \oplus \dots$ that

$$\xi \cdot R_s l_k = \xi \cdot P_j R_s P_0 l_k = \frac{t^j}{j!} \xi \cdot P_j F_j P_0 l_k + O(t^{j+1}) \quad (3.4.86)$$

Now lets directly insert this into the equation (3.4.75) for D_t . We have that

$$D_t(\xi) = \sum_{k=1}^K \int_0^t \frac{s^{2j}}{(j!)^2} |\xi \cdot F^j l_k|^2 + O(s^{2j+1}) ds \quad (3.4.87)$$

which upon integrating gives

$$D_t(\xi) = \frac{1}{(2j+1)(j!)^2} \sum_{k=1}^K |\xi \cdot F^j l_k|^2 t^{2j+1} + O(t^{2j+2}). \quad (3.4.88)$$

Since we have the same relation for R_t^\sharp this relation also holds for D_t^\sharp and we can determine similar results for C_t and C_t^\sharp . Note in particular that in (3.4.87) that taking $s \rightarrow -s$ does not affect the leading order behaviour, and hence to leading order we have

$$C_t = D_t(1 + O(t)) \quad (3.4.89)$$

completing the proof. \square

Note that in the decoherence estimates 3.2.6 the quadratic form

$$\tilde{C}_t(\xi) = \xi \cdot C_t(I + 2GC_t)^{-1} \xi \quad (3.4.90)$$

appears in the exponent of the exponential and using the methods of proof for the previous theorem we can as well determine the leading order behaviour of \tilde{C}_t .

Proposition 3.4.8. *For $\tilde{C}_t(\xi) = \xi \cdot C_t(I + 2GC_t)^{-1} \xi$ we have that*

$$\tilde{C}_t(\xi) = C_t(\xi)(1 + O(t)) \quad (3.4.91)$$

and in particular if we take $\xi \in V_{j-1}^\perp = W_j \oplus W_{j+1} \oplus \dots \oplus W_{r+1}$ then

$$\tilde{C}_t(\xi) = \frac{1}{(2j+1)(j!)^2} \sum_{k=1}^K |\xi \cdot F^j l_k|^2 t^{2j+1} + O(t^{2j+2}). \quad (3.4.92)$$

Proof. We can expand \tilde{C}_t for small t as

$$\tilde{C}_t = C_t + \sum_{n=1}^{\infty} (-1)^n C_t (GC_t)^n. \quad (3.4.93)$$

Now if we apply the form of the expansion of C_t (3.4.82) we previously determined in the above theorem we immediately get the first term. It remains then to show that

the remaining terms $C_t(GC_t)^n$ are of a higher order in t for $n = 1, 2, \dots$. Assume that we have $\xi \in V_{j-1}^\perp$ as in the proposition. Then for any $\eta \in \mathbb{R}^{2n}$ we have

$$\eta \cdot C_t \xi = \sum_k \int_0^t \langle \eta, e^{-sA} l_k \rangle \langle \xi, e^{-sA} l_k \rangle = O(t^{j+1}). \quad (3.4.94)$$

Here we have used the fact that $\langle \eta, e^{-sA} l_k \rangle = O(1)$ and $\langle \xi, e^{-sA} l_k \rangle = O(s^j)$ which follows from lemma 3.4.6. But we took η to be arbitrary and hence this means that $C_t \xi$ must be $O(t^{j+1})$. Using this with $C_t = O(t)$ we get that

$$\xi C_t (GC_t)^n \xi = (C_t \xi) \cdot (GC_t)^{n-1} GC_t \xi = O(t^{2j+1+n}) \quad (3.4.95)$$

completing the proof. \square

Finally, in the following theorem we summarize the relationship between the Hörmander condition and the spread of decoherence.

Theorem 3.4.9 (The Hörmander condition and Decoherence).

For linear Lindblad operators and quadratic Hamiltonians, if the Hörmander condition is satisfied by the vector fields X_j given by (3.3.5) then the system experiences full decoherence. If the Hörmander condition is not satisfied then there exists a decoherence free subspace of \mathbb{R}^{2n} which is protected from the influence of the environment.

Proof. Recall from Theorem 3.2.1 that for linear Lindblads and quadratic Hamiltonians the time evolved characteristic function was given by

$$\chi(t, \xi) = \chi_0(R_t^T \xi) e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi}. \quad (3.4.96)$$

The highly oscillatory terms signifying quantum coherence in the density operator $\hat{\rho}_t$ manifest themselves as large values in the characteristic function since the two are related by Fourier transform. Decoherence is then signified by the decay described by $D_t(\xi) = \xi \cdot D_t \xi$. If D_t is non-degenerate, then this occurs no matter what choice of ξ we choose we see decoherence. However, if D_t is degenerate, then $D_t(\xi)$ has a Kernel in which decoherence does not occur.

By our previous discussion, we know that we can decompose our vector space \mathbb{R}^{2n} into the following orthogonal decomposition:

$$\mathbb{R}^{2n} = W_0 \oplus W_1 \oplus \dots \oplus W_r \oplus W_{df} \quad (3.4.97)$$

where in particular W_{df} is the decoherence free subspace. Using (3.4.75) we have, expanding R_s in the integrand

$$\xi \cdot R_s l_k = \sum_{j=0}^{\infty} \frac{1}{j!} s^j \xi \cdot (F + N\Omega)^j l_k. \quad (3.4.98)$$

Now, since $l_k \in W_0$, the image of N is in W_0 and F can only map into the space $W_0 \oplus \dots \oplus W_r$, we have that

$$(F + N\Omega)^s l_k \in W_{df}^\perp. \quad (3.4.99)$$

Hence, if we take $\xi \in W_{df}$ then the inner product

$$\xi \cdot R_s l_k = 0 \quad (3.4.100)$$

for all $s \in \mathbb{R}$ and so $D_t(\xi) = 0$ for all $t > 0$.

To relate this back now to our definition of decoherence Definition 3.4.1 we consider

$$\rho(t, x) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} x \cdot \xi} \chi(t, \xi) d\xi \quad (3.4.101)$$

which implies

$$|\partial_x^\alpha \rho(t, x)| \leq \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} \frac{1}{\hbar^{|\alpha|}} |\xi^\alpha \chi(t, \xi)| d\xi \quad (3.4.102)$$

$$\leq \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} \frac{1}{\hbar^{|\alpha|}} |\xi|^{|\alpha|} |\chi(0, R_t^T \xi)| e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} d\xi \quad (3.4.103)$$

$$\leq \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} \frac{1}{\hbar^{|\alpha|}} |\xi|^{|\alpha|} \text{tr} |\hat{\rho}_0| e^{-\frac{1}{2\hbar} \xi \cdot D_t \xi} d\xi \quad (3.4.104)$$

using the definition of the characteristic function (2.5.20) and the unitarity of $\hat{T}(\xi)$. Now taking $\xi \rightarrow \sqrt{\hbar} \xi$ we have

$$|\partial_x^\alpha \rho(t, x)| \leq \frac{\hbar^{-\frac{|\alpha|}{2}}}{(2\pi)^n} \int_{\mathbb{R}^{2n}} |\xi|^{|\alpha|} \text{tr} |\hat{\rho}_0| e^{-\frac{1}{2} \xi \cdot D_t \xi} d\xi \quad (3.4.105)$$

$$\leq C_{\alpha, T} \hbar^{-\frac{|\alpha|}{2}} \quad (3.4.106)$$

for a constant $C_{\alpha, T}$ if $D_t(\xi)$ is non-degenerate, which implies that $\rho(t, x) \in S_{\frac{1}{2}}^0$ as required. \square

Chapter 4

Networks of harmonic oscillators as a model of decoherence spread

In this chapter we will focus on some applications of the theory of the previous chapter to a set of examples with particularly nice properties, motivated initially by the example of a chain of interacting harmonic oscillators.

4.1 The motivating example: a chain of harmonic oscillators

We start by recalling example (iv) in Examples 3.4.3 where we chose a system of 2 harmonic oscillators with a nearest neighbour Hooke-like interaction and generalise it.

Take a system composed of N subsystems of the same dimension in phase space such that each individual subsystem is described by a momentum and position $x_k = (q_k, p_k)$. We can think of this as a system of N particles. In this set-up, the system evolves under a Hamiltonian $H(x) = H(q_1, p_1, q_2, p_2, \dots, q_N, p_N)$ which describes both the internal Hamiltonian of each harmonic oscillator as well as the interactions between them. We can think of this as a modelling interacting particles, where for instance, each particle is individually described by a harmonic oscillator. This is a common model chosen in many situations in quantum physics[23][43][26][19][39], molecular chemistry[10] and biophysics[45].

If we directly expand extend out example (iv) in Examples 3.4.3 to an N dimensional system, we have the following Hamiltonian in terms of the creation and annihilation operators \hat{a}^\dagger and \hat{a}

$$\hat{H} = \sum_{i=1}^N \omega_i \hat{a}_i^\dagger \hat{a}_i + \sum_{i=1}^{N-1} \delta_{i,i+1} \left(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_{i+1}^\dagger \hat{a}_i \right) \quad (4.1.1)$$

which can be thought of as describing a chain of interacting oscillators so that the i th oscillator raises and lowers energy levels with its nearest neighbours, governed by the interaction parameter $\delta_{i,i+1}$ and $\delta_{i-1,i}$. If we now write this in the phase space picture

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we have

$$H = \frac{1}{2} \mathbf{x} \cdot H'' \mathbf{x} = \sum_{i=1}^N \omega_i (q_i^2 + p_i^2) + 2 \sum_{i=1}^{N-1} \delta_{i,i+1} (q_i q_{i+1} + p_i p_{i+1}). \quad (4.1.2)$$

In this case, we can write the Hessian of the overall Hamiltonian in block form as

$$H'' = \begin{pmatrix} \omega_1 I & \delta_{12} I & 0 & \cdots & 0 \\ \delta_{12} I & \omega_2 I & \delta_{23} I & & \vdots \\ 0 & \delta_{23} I & \omega_3 I & \ddots & 0 \\ \vdots & & \ddots & \ddots & \delta_{N-1N} I \\ 0 & \cdots & 0 & \delta_{N-1N} I & \omega_N I \end{pmatrix} \quad (4.1.3)$$

Where the ω_i are the frequencies of the internal HO Hamiltonians for each system and the δ_{ii+1} are the interaction parameters between the i th and $(i+1)$ st system (note that this interaction goes both ways). Clearly the above description allows for more complicated networks of particles where particles interact with multiple other particles at once in varying ways.

As well as describing the internal dynamics of the system we also wish to describe how it interacts with the environment. In Example (iv) in (3.4.3) we considered a scattering environment, and we saw that the propagation of decoherence through the system involved some fairly non-trivial subspaces of \mathbb{R}^4 for a system of two interacting oscillators. Now let's instead choose a heat bath model [1] where our Lindblad operators are given by creation and annihilation operators coupled to individual subsystems. That is, we take

$$L_j^c = \gamma_j (q_j - ip_j) \quad (4.1.4)$$

$$L_j^a = \mu_j (q_j + ip_j), \quad (4.1.5)$$

with $\gamma_j, \mu_j \in \mathbb{R}$. Note that as discussed previously the ratio of these two parameters is related to the temperature of the heat bath (see (2.2.73)). In this case, we can write the vectors l_j^c and l_j^a associated to these Lindblad operators as

$$l_j^c = \begin{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \vdots \\ \gamma_j \begin{pmatrix} i \\ 1 \end{pmatrix} \\ \vdots \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix} \quad \text{and} \quad l_j^a = \begin{pmatrix} \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\ \vdots \\ \mu_j \begin{pmatrix} -i \\ 1 \end{pmatrix} \\ \vdots \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} \end{pmatrix}, \quad (4.1.6)$$

where we have abused notation somewhat to indicate the separation of the individual subsystems. We see then that although our system is $2N$ dimensional, nearly all of the useful information is contained in the description of how the N oscillators interact with each other and with the environment. This suggests that we may be able to reduce this $2N$ -dimensional problem to a N -dimensional one. To this end we will introduce the concept of a *Kronecker Product*. This is a generalization of the outer product for vectors and gives a matrix representation of the tensor product[35].

4.1.1 The Kronecker product

Definition 4.1.1 (The Kronecker product). Given an $M \times N$ matrix A and a $m \times n$ matrix B , then the *Kronecker product* denoted by $A \otimes B$ is an $Mm \times Nn$ matrix given in block form by

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1N}B \\ \vdots & \ddots & \vdots \\ a_{M1}B & \cdots & a_{MN}B \end{pmatrix}. \quad (4.1.7)$$

This product has a few important properties which we will need.

Proposition 4.1.2 (Properties of the Kronecker product).

We have the following properties:

(i) *The Kronecker product is bilinear and associative.*

(ii) *It is non-commutative, that is, in general*

$$A \otimes B \neq B \otimes A. \quad (4.1.8)$$

(iii) *For appropriately sized matrices A, B, C, D we have*

$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD). \quad (4.1.9)$$

(iv) *If A and B are invertible matrices, then the matrix $A \otimes B$ is invertible and given by*

$$(A \otimes B)^{-1} = A^{-1} \otimes B^{-1}. \quad (4.1.10)$$

(v) *Similarly, both the transpose and complex conjugation are distributive so that*

$$(A \otimes B)^T = A^T \otimes B^T, \quad (A \otimes B)^* = A^* \otimes B^*. \quad (4.1.11)$$

(vi) *If A is an $N \times N$ matrix with eigenvalues $\lambda_i, i = 1, \dots, N$ and B is an $m \times m$ matrix with eigenvalues $\sigma_j, j = 1, \dots, m$, then the eigenvalues of $A \otimes B$ are given by*

$$\lambda_i \sigma_j \quad \text{for } i = 1, \dots, N, j = 1, \dots, m. \quad (4.1.12)$$

It follows then that

$$\det(A \otimes B) = (\det A)^m (\det B)^N. \quad (4.1.13)$$

and

$$\text{tr}(A \otimes B) = \text{tr } A \text{tr } B. \quad (4.1.14)$$

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4.1.2 Applying the Kronecker product to a chain of harmonic oscillators

In the case of the motivating example, where we have a chain of N coupled harmonic oscillators with nearest neighbour interactions, we can write the Hessian H'' as

$$H'' = \mathbb{H} \otimes I_2 \quad (4.1.15)$$

where I_2 is the 2×2 identity matrix and \mathbb{H} is the $N \times N$ matrix describing the internal frequencies and interaction weights of the system. In particular then we would write

$$H'' = \begin{pmatrix} \omega_1 & \delta_{12} & 0 & \cdots & 0 \\ \delta_{12} & \omega_2 & \delta_{23} & & \vdots \\ 0 & \delta_{23} & \omega_3 & \ddots & 0 \\ \vdots & & \ddots & \ddots & \delta_{N-1N} \\ 0 & \cdots & 0 & \delta_{N-1N} & \omega_N \end{pmatrix} \otimes I_2. \quad (4.1.16)$$

Note that this clearly relies on the symmetry in how we chose our internal Hamiltonians and our interactions, in particular that we can partition our Hessian H into block form where each block is proportional to the identity matrix I_2 .

We can also use this Kronecker product form for the Lindblad terms, where we write the vectors as

$$l_j^c = \mathbb{I}_j^c \otimes \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad l_j^a = \mathbb{I}_j^a \otimes \begin{pmatrix} -i \\ 1 \end{pmatrix} \quad (4.1.17)$$

so in the above we would have

$$l_j^c = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \gamma_j \\ 0 \\ \vdots \\ 0 \end{pmatrix} \otimes \begin{pmatrix} i \\ 1 \end{pmatrix}, \quad l_j^a = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \mu_j \\ 0 \\ \vdots \\ 0 \end{pmatrix} \otimes \begin{pmatrix} -i \\ 1 \end{pmatrix}. \quad (4.1.18)$$

From Theorem 3.4.9 we know that the spread of decoherence is intimately related to Hörmander's condition. Recall that for linear Lindblad operators and a quadratic Hamiltonian that we saw in (2.6.24) that A was given by

$$A = \Omega H'' + N\Omega = F + N\Omega \quad (4.1.19)$$

where F is the Hamiltonian map $F = \Omega H''$ and N and M could be related to the l_j 's via

$$\sum_j \bar{l}_j l_j^T = M + iN.$$

Since we are dealing with N systems, we have that Ω is of the form

$$\Omega = \begin{pmatrix} \Omega_2 & & 0 \\ & \ddots & \\ 0 & & \Omega_2 \end{pmatrix} = I_N \otimes \Omega_2. \quad (4.1.20)$$

Lets take the most general case, where we have a creation and annihilation operator for each subsystem with (possibly zero) weights γ_j and μ_j , for a total of $2N$ Lindblad operators. In this case we have

$$\sum_{j=1}^N \bar{l}_j^c (l_j^c)^T + \bar{l}_j^a (l_j^a)^T = M + iN. \quad (4.1.21)$$

Computing this, we have

$$\begin{aligned} M + iN &= \sum_j \bar{l}_j^c (l_j^c)^T \otimes \begin{pmatrix} -i \\ 1 \end{pmatrix} \begin{pmatrix} i & -1 \end{pmatrix} + \bar{l}_j^a (l_j^a)^T \otimes \begin{pmatrix} i \\ 1 \end{pmatrix} \begin{pmatrix} -i & -1 \end{pmatrix} \\ &= \begin{pmatrix} \gamma_1^2 & & 0 \\ & \gamma_2^2 & \\ & & \ddots \\ 0 & & & \gamma_N^2 \end{pmatrix} \otimes \begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} + \begin{pmatrix} \mu_1^2 & & 0 \\ & \mu_2^2 & \\ & & \ddots \\ 0 & & & \mu_N^2 \end{pmatrix} \otimes \begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \\ &= \begin{pmatrix} \gamma_1^2 + \mu_1^2 & & 0 \\ & \ddots & \\ 0 & & \gamma_N^2 + \mu_N^2 \end{pmatrix} \otimes I_2 + i \begin{pmatrix} \mu_1^2 - \gamma_1^2 & & 0 \\ & \ddots & \\ 0 & & \mu_N^2 - \gamma_N^2 \end{pmatrix} \otimes \Omega_2 \\ &= \mathbb{M} \otimes I_2 + i\mathbb{N} \otimes \Omega_2. \end{aligned} \quad (4.1.22)$$

Using this and the results we had for H'' and Ω , we have that

$$\begin{aligned} A &= \Omega H'' + N\Omega \\ &= (I_N \otimes \Omega_2)(\mathbb{H} \otimes I_2) + (\mathbb{N} \otimes \Omega_2)(I_N \otimes \Omega_2) \\ &= \mathbb{H} \otimes \Omega_2 - \mathbb{N} \otimes I_2. \end{aligned} \quad (4.1.23)$$

Recall now the specific form of the Hörmander condition we determined in (3.4.2) and that we also introduced an orthogonal decomposition of the subspaces V_k such that

$$V_k = W_0 \oplus \dots \oplus W_k \quad (4.1.24)$$

where $W_i \perp W_j$ for $i \neq j$.

We saw in Examples 3.4.3 that the choice where we have $2N$ linearly independent Lindblad operators was not particularly interesting, since the Hörmander condition is immediately satisfied since $V_0 \cong \mathbb{R}^{2N}$. Perhaps more interesting then is the case we touched on before where we only have one set of Lindblad operators and we wish to see whether the internal dynamics of the system will carry the decoherence induced by this

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coupling to all degrees of freedom. This would correspond to taking $\gamma_j, \mu_j = 0$ for all but a single choice of j .

Let's consider the most basic case of a chain of 3 harmonic oscillators coupled to a heat bath environment to see how, by using the Kronecker product, we can simplify the method of checking Hörmander's condition, and investigate how the macro structure of the system affects the spread of decoherence.

Example 4.1.3 (A chain of 3 oscillators: First oscillator environment coupling). We consider the case where we have a chain of 3 harmonic oscillators with the same frequency ω and the same interaction parameter δ . Let's couple our Lindblad operators to the first harmonic oscillator. This is shown diagrammatically in Fig 4.1

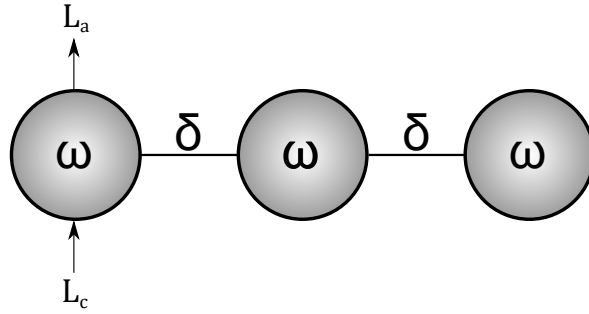


Figure 4.1: A chain of 3 harmonic oscillators with the same frequency ω and interaction δ . We couple the heat bath to the first oscillator, indicated by a creation operator pumping energy into the system and an annihilation operator pumping energy out of the system.

In this case we have, using the previous results:

$$H'' = \begin{pmatrix} \omega & \delta & 0 \\ \delta & \omega & \delta \\ 0 & \delta & \omega \end{pmatrix} \otimes I_2, \quad (4.1.25)$$

and thus, using (4.1.9)

$$F = \Omega H'' = \begin{pmatrix} \omega & \delta & 0 \\ \delta & \omega & \delta \\ 0 & \delta & \omega \end{pmatrix} \otimes \Omega_2 = \mathbb{H} \otimes \Omega_2. \quad (4.1.26)$$

We also have the Lindblad vectors

$$l^c = \gamma \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} i \\ 1 \end{pmatrix} \quad (4.1.27)$$

$$l^a = \mu \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} -i \\ 1 \end{pmatrix}. \quad (4.1.28)$$

Hence,

$$\operatorname{Re} l^c = \gamma \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \operatorname{Re} l^a = \mu \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (4.1.29)$$

$$\operatorname{Im} l^c = \gamma \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \operatorname{Im} l^a = -\mu \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (4.1.30)$$

From this it is straightforward to see that

$$V_0 = W_0 = \operatorname{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{e}_1, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{e}_2 \right\} = \mathbb{R}^2 \subset \mathbb{R}^6, \quad (4.1.31)$$

where we have defined

$$\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (4.1.32)$$

Clearly then the Hörmander condition is not satisfied yet and we need to go to higher terms. Recall that

$$V_1 = V_0 + FV_0. \quad (4.1.33)$$

Thus,

$$FV_0 = \operatorname{span} \left\{ (\mathbb{H} \otimes \Omega_2) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{e}_1, (\mathbb{H} \otimes \Omega_2) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{e}_2 \right\} \quad (4.1.34)$$

$$= \operatorname{span} \left\{ \begin{pmatrix} \omega \\ \delta \\ 0 \end{pmatrix} \otimes \mathbf{e}_2, \begin{pmatrix} \omega \\ \delta \\ 0 \end{pmatrix} \otimes -\mathbf{e}_1 \right\}. \quad (4.1.35)$$

Clearly then, since \mathbf{e}_1 and \mathbf{e}_2 are linearly independent, and $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} \omega \\ \delta \\ 0 \end{pmatrix}$ are linearly independent, we have that

$$V_1 = V_0 + FV_0 \cong \mathbb{R}^4 \subset \mathbb{R}^6. \quad (4.1.36)$$

Indeed we can see immediately that the orthogonal subspace W_1 is given by

$$W_1 = \operatorname{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{e}_1, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{e}_2 \right\}. \quad (4.1.37)$$

Continuing, we have

$$V_2 = V_0 + FV_0 + F^2V_0, \quad (4.1.38)$$

$$F^2V_0 = \text{span} \left\{ (\mathbb{H} \otimes \Omega_2) \begin{pmatrix} \omega \\ \delta \\ 0 \end{pmatrix} \otimes \mathbf{e}_1, (\mathbb{H} \otimes \Omega_2) \begin{pmatrix} \omega \\ \delta \\ 0 \end{pmatrix} \otimes \mathbf{e}_2 \right\} \quad (4.1.39)$$

$$= \text{span} \left\{ \begin{pmatrix} \omega^2 + \delta^2 \\ 2\omega\delta \\ \delta^2 \end{pmatrix} \otimes \mathbf{e}_2, \begin{pmatrix} \omega^2 + \delta^2 \\ 2\omega\delta \\ \delta^2 \end{pmatrix} \otimes -\mathbf{e}_1 \right\}. \quad (4.1.40)$$

Clearly, $\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$, $\begin{pmatrix} \omega \\ \delta \\ 0 \end{pmatrix}$ and $\begin{pmatrix} \omega^2 + \delta^2 \\ 2\omega\delta \\ \delta^2 \end{pmatrix}$ are all linearly independent and hence

$$V_2 = V_0 + FV_0 + F^2V_0 \cong \mathbb{R}^6 \quad (4.1.41)$$

and Hörmander's condition is satisfied. Thus decoherence introduced by the Lindblad operators at the first particle will spread throughout the system. Indeed if we investigate the W spaces, we see immediately that, using the notation $\mathbf{e}_{1,2}$ for simplicity,

$$W_0 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \otimes \mathbf{e}_{1,2} \right\}, \quad W_1 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{e}_{1,2} \right\}, \quad W_2 = \text{span} \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \otimes \mathbf{e}_{1,2} \right\}. \quad (4.1.42)$$

These are clearly just the subspaces corresponding to the individual oscillators, so we see that the effect of decoherence spreads down the chain as we might expect, so that the oscillator furthest away from the noise decoheres last. If we place cat states in the subspaces corresponding to each of the oscillators, and investigate the Hilbert-Schmidt norm of the cross terms as we did previously in Example. ??, we see the separation of timescales as predicted, shown in Fig. 4.2.

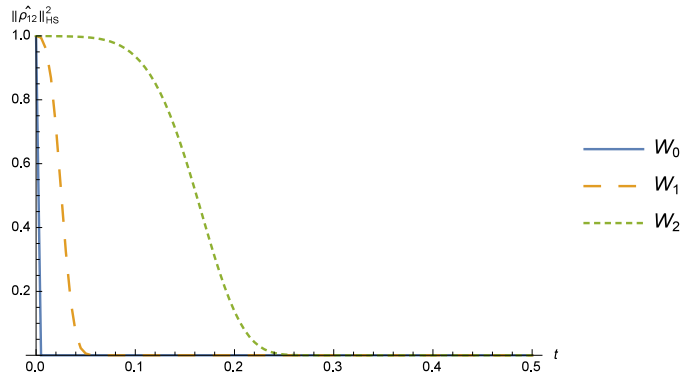


Figure 4.2: The Hilbert-Schmidt norm of $\rho_{12}(t, x)$ in Lemma 3.2.6 for a chain of three Harmonic oscillators and a heat bath environment coupled to the first oscillator initialised in the subspaces W_0, W_1 and W_2 for $\hbar = 10^{-5}$, $\omega = 1$, $\delta = 1$, $\mu = 0.1$, $\gamma = 0.05$. Note that timelag in the onset of the decoherence.

Example 4.1.4 (A chain of 3 oscillators: Middle oscillator environment coupling). Now let's change things just slightly by now coupling the Lindblad's instead to the middle particle.

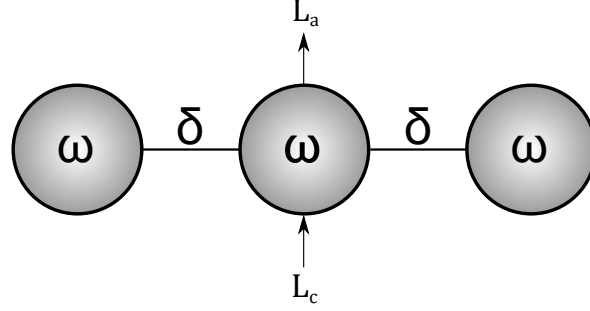


Figure 4.3: A chain of 3 harmonic oscillators with the same frequency ω and interaction δ . We couple the heat bath to the middle oscillator, indicated by a creation operator pumping energy into the system and an annihilation operator pumping energy out of the system.

Then we can quickly repeat the above calculations to get

$$V_0 = W_0 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{e}_1, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{e}_2 \right\}, \quad (4.1.43)$$

$$FV_0 = \text{span} \left\{ \begin{pmatrix} \delta \\ \omega \\ \delta \end{pmatrix} \otimes \mathbf{e}_1, \begin{pmatrix} \delta \\ \omega \\ \delta \end{pmatrix} \otimes \mathbf{e}_2 \right\} \quad (4.1.44)$$

and

$$F^2V_0 = \text{span} \left\{ \begin{pmatrix} 2\delta\omega \\ \omega^2 + 2\delta^2 \\ 2\delta\omega \end{pmatrix} \otimes \mathbf{e}_1, \begin{pmatrix} 2\delta\omega \\ \omega^2 + 2\delta^2 \\ 2\delta\omega \end{pmatrix} \otimes \mathbf{e}_2 \right\}. \quad (4.1.45)$$

If we test for linear independence with these 3 vectors now, using the determinant, then we have,

$$\det \begin{pmatrix} 0 & \delta & 2\delta\omega \\ 1 & \omega & \omega^2 + 2\delta^2 \\ 0 & \delta & 2\delta\omega \end{pmatrix} = -\det \begin{pmatrix} \delta & 2\delta\omega \\ \delta & 2\delta\omega \end{pmatrix} = 0 \quad (4.1.46)$$

and hence the 3 vectors are not linearly independent. Thus

$$V_2 = V_0 + FV_0 + F^2V_0 = V_1 \cong \mathbb{R}^4. \quad (4.1.47)$$

Hence there is a violation of Hörmander's condition. In terms of decoherence, this means there is some subspace of the system which is insulated from the effect of the coupling of the Lindblads and does not experience decoherence. Recall that this was simply a result of changing which particle in the chain we coupled the environment to.

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If we compute the orthogonal decomposition into the W subspaces for this system, we find that

$$W_0 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \otimes \mathbf{e}_{1,2} \right\}, \quad W_1 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \otimes \mathbf{e}_{1,2} \right\}, \quad W_{df} = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \otimes \mathbf{e}_{1,2} \right\} \quad (4.1.48)$$

where as before we have used the notation W_{df} to indicate the decoherence free subspace. If we compute the Hilbert-Schmidt norms for cat states centred in these subspaces, we again see that the decoherence free subspace is insulated from the environment, as is shown in Fig. 4.4.

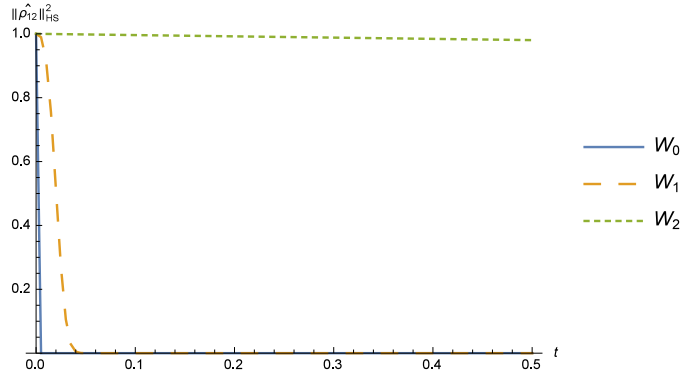


Figure 4.4: The Hilbert-Schmidt norm of $\rho_{12}(t, x)$ in Lemma 3.2.6 for a chain of three Harmonic oscillators and a heat bath environment coupled to the middle oscillator initialised in the subspaces W_0, W_1 and $W_2 = W_{df}$ for $\hbar = 10^{-5}$, $\omega = 1$, $\delta = 1$, $\mu = 0.1$, $\gamma = 0.05$. Note that timelag in the onset of the decoherence and that the decoherence free subspace is insulated.

4.1.3 Advantages of the model

We now summarize the main advantages of this model that allowed us to simplify our problem.

Firstly, the fact that our matrix H'' could be reduced to the form $H'' = \mathbb{H} \otimes I_2$ meant that we could reduce our problem to considering products of N dimensional rather than $2N$ dimensional matrices.

Secondly, the fact that our choice of Lindblad operators spanned the subspace of an individual system, or more precisely their real and imaginary parts spanned the subspace, meant that applying $F = \mathbb{H} \otimes \Omega_2$ to these vectors would produce a set of vectors that also spanned the space. Note that in this case the choice of creation and annihilation operators is not unique in this, indeed any set of non-zero vectors $v_1, v_2 \in \mathbb{R}^2$ such that $v_1 \cdot v_2 = 0$ would satisfy this since $\Omega v_1 \cdot \Omega v_2 = v_1 \cdot \Omega^T \Omega v_2 = v_1 \cdot v_2 = 0$.

The result of this is that we only need to consider the system and environment on a macro level with the structure of the system of coupled harmonic oscillators described

by the matrix \mathbb{H} , and the coupling to the environment, described by a coupling vector which we will denote by \mathfrak{c} . We summarise this in the following lemma.

Lemma 4.1.5 (A specific Hörmander condition). *Suppose we have a network of coupled harmonic oscillators with a heat bath coupling described by (4.1.4) and (4.1.5) with the vector form (4.1.17). Writing*

$$V_k = \mathbb{V}_k \otimes \mathbb{R}^2, \quad (4.1.49)$$

the Hörmander condition (3.4.2) holds if and only if $\mathbb{V}_k = \mathbb{R}^N$ for some $k \leq N - 1$.

Proof. From (3.4.2) V_0 is defined as

$$V_0 = \text{span}\{\text{Re } l_k, \text{Im } l_k, k = 1, \dots, K\} \quad (4.1.50)$$

which for (4.1.17) gives

$$\begin{aligned} V_0 &= \text{span}\{\mathbb{I}_j^c, \mathbb{I}_j^a, j = 1, \dots, N\} \otimes \mathbb{R}^2 \\ &= \mathbb{V}_0 \otimes \mathbb{R}^2. \end{aligned} \quad (4.1.51)$$

Now

$$F = \mathbb{H} \otimes \Omega_2 \quad (4.1.52)$$

and hence $V_1 = V_0 + FV_0$ where

$$FV_0 = \mathbb{H}\mathbb{V}_0 \otimes \Omega_2 \mathbb{R}^2 = \mathbb{H}\mathbb{V}_0 \otimes \mathbb{R}^2. \quad (4.1.53)$$

Extending this we have

$$\begin{aligned} V_k &= FV_{k-1} + V_{k-1} \\ &= \mathbb{H}\mathbb{V}_{k-1} \otimes \mathbb{R}^2 + \mathbb{V}_{k-1} \otimes \mathbb{R}^2 \\ &= \mathbb{V}_k \otimes \mathbb{R}^2 \end{aligned} \quad (4.1.54)$$

and hence we see that Hörmander's condition holds if and only if $\mathbb{V}_k = \mathbb{R}^N$ for some $k \leq N - 1$. \square

The matrix \mathbb{H} has a lot of similarities to the adjacency matrices of graph theory since it describes the connections between oscillators. However it is not quite the same since it has a non-zero diagonal component and the elements are not integers describing the number of connections but weights describing the interactions and internal hamiltonians of the subsystems. However, as long as the interactions between the subsystems are undirected, then the matrix \mathbb{H} is symmetric and hence diagonalizable with real eigenvalues.

Let's use these simplifications to investigate the spread of decoherence in a chain of N harmonic oscillators.

4.1.4 When does Hörmander's condition fail?

We start by re-analysing our simple example of a chain of 3 oscillators. We have that the matrix \mathbb{H} is given by

$$\mathbb{H} = \begin{pmatrix} \omega & \delta & 0 \\ \delta & \omega & \delta \\ 0 & \delta & \omega \end{pmatrix} \quad (4.1.55)$$

and we showed that for the choice of first particle environment coupling, corresponding to a coupling vector we denote by \mathfrak{c}

$$\mathfrak{c} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad (4.1.56)$$

the Hörmander condition was satisfied. However, if instead we chose

$$\mathfrak{c} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (4.1.57)$$

it was not. We saw that checking this basically boiled down to checking whether the vectors

$$\mathfrak{c}, \mathbb{H}\mathfrak{c}, \mathbb{H}^2\mathfrak{c} \quad (4.1.58)$$

were linearly independent.

If we now consider the N oscillator case, with \mathbb{H} given by (4.1.16) with $\omega_j = \omega$ and $\delta_{jk} = \delta, \forall j, k$, and with \mathfrak{c} now an N dimensional vector, we can clearly extend this idea. We require that the vectors

$$\mathfrak{c}, \mathbb{H}\mathfrak{c}, \mathbb{H}^2\mathfrak{c}, \dots, \mathbb{H}^{N-1}\mathfrak{c} \quad (4.1.59)$$

need to be linearly independent. Note then that we can check this condition simply by checking that the determinant

$$\det C = \det (\mathfrak{c}, \mathbb{H}\mathfrak{c}, \mathbb{H}^2\mathfrak{c}, \dots, \mathbb{H}^{N-1}\mathfrak{c}) \neq 0 \quad (4.1.60)$$

where we have denoted the matrix whose columns are given by the vectors above by C .

Let us use the fact that \mathbb{H} is symmetric and hence diagonalizable, and write \mathbb{H} as it's spectral decomposition

$$\mathbb{H} = \sum_{i=1}^N \lambda_i |v_i\rangle \langle v_i| \quad (4.1.61)$$

Let's also write \mathfrak{c} in this basis

$$\mathfrak{c} = \sum_{j=1}^N c_j |v_j\rangle. \quad (4.1.62)$$

Then,

$$\mathbb{H}^j \mathfrak{c} = \sum_{i=1}^N \lambda_i^j c_i |v_i\rangle \quad (4.1.63)$$

for $j = 0, \dots, N-1$. Then in this basis, the matrix C is given simply by

$$C = \begin{pmatrix} c_1 & \lambda_1 c_1 & \cdots & \lambda_1^{N-1} c_1 \\ c_2 & \lambda_2 c_2 & \cdots & \lambda_2^{N-1} c_2 \\ \vdots & \vdots & \ddots & \vdots \\ c_N & \lambda_N c_N & \cdots & \lambda_N^{N-1} c_N \end{pmatrix}. \quad (4.1.64)$$

We can write this as the product of two matrices

$$C = \begin{pmatrix} c_1 & 0 & \cdots & 0 \\ 0 & c_2 & & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \cdots & 0 & c_N \end{pmatrix} \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{N-1} \\ 1 & \lambda_2 & \cdots & \lambda_2^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N & \cdots & \lambda_N^{N-1} \end{pmatrix}. \quad (4.1.65)$$

The matrix on the right is in the well known form of a *Vandermonde Matrix* which is particularly useful because it has a well known and simple determinant [21] given by

$$\det \begin{pmatrix} 1 & \lambda_1 & \cdots & \lambda_1^{N-1} \\ 1 & \lambda_2 & \cdots & \lambda_2^{N-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \lambda_N & \cdots & \lambda_N^{N-1} \end{pmatrix} = \prod_{1 \leq j < k \leq N} (\lambda_k - \lambda_j). \quad (4.1.66)$$

Since $\det AB = \det A \det B$ we can thus reduce our condition (4.1.60) to requiring that

$$\det C = \prod_i c_i \prod_{1 \leq j < k \leq N} (\lambda_k - \lambda_j) \neq 0. \quad (4.1.67)$$

We see then that if \mathbb{H} is chosen degenerate, then the Vandermonde determinant product is zero (since $\lambda_k = \lambda_j$ for $j \neq k$) and Hörmander's condition fails for *all* choices of \mathfrak{C} .

For \mathbb{H} chosen non-degenerate we need to check that all the c_i 's, that is the coefficients of \mathfrak{c} in the eigenbasis of \mathbb{H} , are non-zero. This makes sense intuitively since we need the effect of the coupling to the environment to reach all parts of the system.

Let's check this condition against the two examples we considered above for a chain of 3 oscillators. We had, in the standard basis, which we will denote by \mathbf{e} :

$$\mathbb{H} = \begin{pmatrix} \omega & \delta & 0 \\ \delta & \omega & \delta \\ 0 & \delta & \omega \end{pmatrix}_{\mathbf{e}} \quad (4.1.68)$$

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The eigenvalues of \mathbb{H} are, with associated normalized eigenvectors:

$$\lambda_1 = \omega, \quad \mathbf{v}_1 = \frac{1}{2} \begin{pmatrix} \sqrt{2} \\ 0 \\ -\sqrt{2} \end{pmatrix} \quad (4.1.69)$$

$$\lambda_2 = \omega + \sqrt{2}\delta, \quad \mathbf{v}_2 = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \quad (4.1.70)$$

$$\lambda_3 = \omega - \sqrt{2}\delta, \quad \mathbf{v}_3 = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}. \quad (4.1.71)$$

Thus the transformation matrix is

$$P = \frac{1}{2} \begin{pmatrix} \sqrt{2} & 1 & 1 \\ 0 & -\sqrt{2} & \sqrt{2} \\ -\sqrt{2} & 1 & 1 \end{pmatrix} \quad (4.1.72)$$

and its inverse is

$$P^{-1} = \frac{1}{2} \begin{pmatrix} \sqrt{2} & 0 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \\ 1 & \sqrt{2} & 1 \end{pmatrix}. \quad (4.1.73)$$

Hence,

$$\mathbb{C}_{\mathbf{v}} = P^{-1} \mathbb{C}_{\mathbf{e}}. \quad (4.1.74)$$

So, for

$$\mathbb{C}_{\mathbf{e}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad (4.1.75)$$

we have

$$\mathbb{C}_{\mathbf{v}} = \frac{1}{2} \begin{pmatrix} \sqrt{2} \\ 1 \\ 1 \end{pmatrix} \quad (4.1.76)$$

and all components are non-zero, thus (4.1.67) is non-zero and Hörmander's condition is satisfied, as expected from our previous work. Now, for the case

$$\mathbb{C}_{\mathbf{e}} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (4.1.77)$$

we have

$$\mathbb{C}_{\mathbf{v}} = \frac{1}{2} \begin{pmatrix} 0 \\ -\sqrt{2} \\ \sqrt{2} \end{pmatrix} \quad (4.1.78)$$

and clearly the first component is zero and (4.1.67) is thus zero and Hörmander's condition is not satisfied. This suggests that the eigenspace of the system corresponding to the first eigenvalue is insulated from the noise introduced by the environment. Indeed if we look, this eigenspace is given by the span of the vector $\mathbf{v}_1 = \frac{1}{2}(\sqrt{2}, 0, -\sqrt{2})^T$ which is exactly the decoherence free subspace W_{df} we found earlier.

In the case of N oscillators, the matrix \mathbb{H} is of the form

$$\mathbb{H} = \begin{pmatrix} \omega & \delta & & 0 \\ \delta & \omega & \delta & \\ & \delta & \omega & \\ & & & \ddots & \delta \\ 0 & & & \delta & \omega \end{pmatrix} \quad (4.1.79)$$

This matrix is in symmetric Toeplitz form. Yueh [50] provides us with some eigenvalue results for the specific case of tridiagonal matrices that we find here. In that paper a slightly more general case is considered where the top left and bottom right entries are allowed to be perturbed by some values α and β and the matrix need not be symmetric. In particular, matrices of the following form are considered:

$$A_N = \begin{pmatrix} -\alpha + b & c & & 0 \\ a & b & c & \\ & a & b & \\ & & & \ddots & c \\ 0 & & & a & -\beta + b \end{pmatrix} \quad (4.1.80)$$

However they do consider the case $\alpha = \beta = 0$ and show that the eigenvalues and eigenvectors of this matrix are given by

$$\lambda_k = b + 2\sqrt{ac} \cos \frac{k\pi}{N+1}, \quad \mathbf{u}^{(k)} = (u_1^{(k)} u_2^{(k)}, \dots, u_N^{(k)})^T \quad (4.1.81)$$

where

$$u_j^{(k)} = \left(\frac{a}{c}\right)^{\frac{j-1}{2}} \sin \frac{kj\pi}{N+1}, \quad j = 1, \dots, N \quad (4.1.82)$$

for $k = 1, \dots, N$. We can then use this in our situation with $a = c = \delta$ and $b = \omega$ to get

$$\lambda_k = \omega + 2\delta \cos \frac{k\pi}{N+1}, \quad \mathbf{u}^{(k)} = \left(\sin \frac{k\pi}{N+1}, \sin \frac{k2\pi}{N+1}, \dots, \sin \frac{kN\pi}{N+1} \right)^T. \quad (4.1.83)$$

Clearly the eigenvalues are all distinct, because $\cos \frac{k\pi}{N+1}$ is strictly decreasing in k for $k = 1, \dots, N$. Thus, the Vandermonde side of the determinant condition (4.1.67) never fails in this case. Thus we can only investigate how the coupling vector might fail.

The matrix P is given by

$$P = \begin{pmatrix} \sin \frac{\pi}{N+1} & \sin \frac{2\pi}{N+1} & \cdots & \sin \frac{N\pi}{N+1} \\ \sin \frac{2\pi}{N+1} & \sin \frac{4\pi}{N+1} & \cdots & \sin \frac{2N\pi}{N+1} \\ \vdots & \vdots & & \vdots \\ \sin \frac{N\pi}{N+1} & \sin \frac{2N\pi}{N+1} & \cdots & \sin \frac{N^2\pi}{N+1} \end{pmatrix} \quad (4.1.84)$$

Now of course, what we really need to find is the inverse of this matrix. We claim that

$$P^2 = \frac{N+1}{2} I_n. \quad (4.1.85)$$

Note that

$$(P^2)_{kl} = \sum_{j=1}^N \sin \frac{kj\pi}{N+1} \sin \frac{lj\pi}{N+1}. \quad (4.1.86)$$

From here we are in the situation of Appendix B and can apply its result

$$\sum_{j=1}^N \sin \left(\frac{k\pi}{N+1} j \right) \sin \left(\frac{l\pi}{N+1} j \right) = \frac{N+1}{2} \delta_{kl} \quad (4.1.87)$$

directly. Given this, we have

$$P^{-1} = \frac{2}{N+1} P. \quad (4.1.88)$$

Now, in keeping with the analysis we did for the 3 particle case, let's look for the zeros that appear in this matrix. The column these zeros appear in corresponds to a choice of an individual oscillator to which coupling the noise will cause only limited decoherence propagation throughout the system. That is, there will be some degrees of freedom untouched by decoherence. Given the form of P we can easily see that

$$\sin \frac{kl\pi}{N+1} = 0 \quad \text{when} \quad \frac{kl\pi}{N+1} = 1 \quad (4.1.89)$$

in the range we are considering. Hence,

$$kl = N+1 \quad (4.1.90)$$

is required. When $N+1$ is prime there is no choice of k and l for which this is the case. Thus we have the interesting result that in the case of a chain of N particles, for $N+1$ non-prime there will always be an individual particle to which you can couple the environment which will leave some part of the system insulated from the decoherence effects. However, in the cases where $N+1$ is prime there is no such choice, and there is complete decoherence throughout the system.

If we were to allow a coupling to multiple subsystems at once then this result would change, and indeed in perhaps the most physically realistic case we would have all oscillators coupled to the environment. However, it is of interest to consider the situation where we have one oscillator coupled more strongly than the rest, in which case the single oscillator environment coupling would be the limiting case.

4.2 Extending the theory

In this section we will indicate how one might extend the method we used in the previous section to investigate the Hörmander condition to more general networks. We will start

by describing the kind of systems we will be dealing with, before then moving on to describing the type of environment we wish to consider and then give the general method for investigating the Hörmander condition and hence the spread of decoherence.

Let us start by stating our assumptions about the systems we wish to consider.

- First and foremost, as before we assume that our overall Hamiltonian $H(x)$ is at most quadratic in x .
- We will assume that our system can be partitioned into N interacting subsystems and that these subsystems are all of the same type. That is, the Hessian of the Hamiltonian of these subsystems is of the same form. For example, we could consider a set of harmonic oscillators with Hessian

$$H'' = \begin{pmatrix} \omega & 0 \\ 0 & \omega \end{pmatrix} \quad (4.2.1)$$

where the ω could be different for each individual subsystem but the structure is the same.

- Similarly, we will assume that all interactions between these subsystems are of the same form and are undirected.

We can arrive at an even more general approach if we relax these assumptions by allowing disparate subsystems and interactions but the majority of the examples we might wish to consider will fall under these assumptions.

Given these assumptions, and given that we can write the Hamiltonian of the full system in the form

$$H = \frac{1}{2} \mathbf{x} \cdot H'' \mathbf{x} \quad (4.2.2)$$

where $\mathbf{x} = (q_1, p_1, q_2, p_2, \dots, q_N, p_N)^T$ we can separate our Hessian matrix into parts describing the internal subsystem dynamics and parts describing the interactions between the subsystems,

$$H'' = \mathbb{H}_S \otimes h_S + \mathbb{H}_I \otimes h_I. \quad (4.2.3)$$

Here h_S and h_I are the Hamiltonian matrices of the individual systems and interactions between systems, and \mathbb{H}_S and \mathbb{H}_I describe the structure and scaling of the subsystems and their interactions. Here, again, we use the Kronecker product to our advantage.

Now lets move on to considering the environment. We make the standard assumption, namely that, as before, the Lindblad operators L_k we consider are linear and can be written in the form

$$L_k = \Omega l_k \cdot \mathbf{x}. \quad (4.2.4)$$

Note that given the form of L_k above, we can write each individual vector l_k in the following form

$$l_k = \mathbb{c}_k \otimes c_k \quad (4.2.5)$$

where c_k is the form of the individual Lindblad vector acting on a subsystem and \mathbb{c}_k is the *coupling vector* which describes to which system or systems the Lindblad operator

is coupled, which we will take to be real. Note that here we are allowing for different forms of Lindblad vectors acting on the individual subsystems, but we will usually find that they are all of similar type.

Given these assumptions, we state the following result which describes a method for checking Hörmander's condition.

Theorem 4.2.1 (An algorithm for checking the Hörmander condition). *Given a quadratic Hamiltonian describing a system composed of interacting subsystems of the same type, and a set of linear Lindblad operators as described above, to check the Hörmander condition, we need to check that the set of vectors*

$$\{F^n \operatorname{Re} l_k, F^n \operatorname{Im} l_k, n = 1, \dots, r\} \quad (4.2.6)$$

are linearly independent for some $r \leq 2N - 1$, where in terms of the expansions (4.2.3) and (4.2.5)

$$F^n \operatorname{Re} l_k = \sum_{i=0}^n \binom{n}{i} [(\mathbb{H}_S)^{n-i} (\mathbb{H}_I)^i c_k] \otimes [(\Omega_2 h_S)^{n-i} (\Omega_2 h_I)^i \operatorname{Re} c_k] \quad (4.2.7)$$

and

$$F^n \operatorname{Im} l_k = \sum_{i=0}^n \binom{n}{i} [(\mathbb{H}_S)^{n-i} (\mathbb{H}_I)^i c_k] \otimes [(\Omega_2 h_S)^{n-i} (\Omega_2 h_I)^i \operatorname{Im} c_k] \quad (4.2.8)$$

where $\binom{n}{i}$ is the standard binomial coefficient.

Proof. This is really a straightforward application of the results of the previous chapter. As we saw, the Hörmander condition in this case reduces to considering the spaces

$$V_0 = \operatorname{span}\{\operatorname{Re} l_k, \operatorname{Im} l_k \mid k = 1, \dots, K\} \subset \mathbb{R}^{2n} \quad (4.2.9)$$

and

$$V_j = V_0 + FV_0 + F^2V_0 + \dots + F^jV_0 \subset \mathbb{R}^{2n}. \quad (4.2.10)$$

In particular we wish to check whether there is an $r \leq 2n - 1$ such that $V_r = \mathbb{R}^{2n}$. For this to be the case, the set of vectors (4.2.6) must be linearly independent for some $r \leq 2n - 1$.

To determine (4.2.7) and (4.2.8) we first use that

$$F = \Omega H'' \quad (4.2.11)$$

where Ω is the standard $2n \times 2n$ symplectic matrix which we can write in tensor form as

$$\Omega = I_n \otimes \Omega_2 \quad (4.2.12)$$

where $\Omega_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

Now, using (4.1.9) we see that, in terms of the expansion of H'' (4.2.3), we can write F as

$$F = \Omega H'' = \mathbb{H}^S \otimes \Omega_2 h^S + \mathbb{H}^I \otimes \Omega_2 h^I. \quad (4.2.13)$$

Now we need the real and imaginary parts of the vectors l_k . Note that we have the following result for the real and imaginary parts of a Kronecker product, which follows from (4.1.11):

$$\operatorname{Re}(A \otimes b) = \operatorname{Re} A \otimes \operatorname{Re} b - \operatorname{Im} A \otimes \operatorname{Im} b, \quad (4.2.14)$$

and

$$\operatorname{Im}(A \otimes b) = \operatorname{Im} A \otimes \operatorname{Re} b + \operatorname{Re} A \otimes \operatorname{Im} b. \quad (4.2.15)$$

Since we chose our coupling vectors c_k to be exclusively real valued then clearly we can simplify things so that

$$\operatorname{Re} l_k = c_k \otimes \operatorname{Re} c_k, \quad \operatorname{Im} l_k = c_k \otimes \operatorname{Im} c_k. \quad (4.2.16)$$

Using this and the form of F we have

$$\begin{aligned} F \operatorname{Re} l_k &= (\mathbb{H}_S \otimes \Omega_2 h_S + \mathbb{H}_I \otimes \Omega_2 h_I) (c_k \otimes \operatorname{Re} c_k) \\ &= (\mathbb{H}_S c_k) \otimes (\Omega_2 h_S \operatorname{Re} c_k) + (\mathbb{H}_I c_k) \otimes (\Omega_2 h_I \operatorname{Re} c_k) \end{aligned} \quad (4.2.17)$$

and similarly for the Imaginary part. Clearly then higher powers of F will be given by a binomial expansion

$$F^n \operatorname{Re} l_k = \sum_{i=0}^n \binom{n}{i} [(\mathbb{H}_S)^{n-i} (\mathbb{H}_I)^i c_k] \otimes [(\Omega_2 h_S)^{n-i} (\Omega_2 h_I)^i \operatorname{Re} c_k] \quad (4.2.18)$$

and again similarly for $\operatorname{Im} l_k$, giving the result. \square

Clearly for general systems this can get pretty complicated but the advantage of this method is that there are often simplifications that allow us to make the calculation easier. For example, if the matrices $h_S = h_I = h$, as was the case in the example of the chain of harmonic oscillators we considered above, then we can simplify to

$$H'' = \mathbb{H} \otimes h \quad (4.2.19)$$

where $\mathbb{H} = \mathbb{H}_S + \mathbb{H}_I$ which is a symmetric matrix. In this case, we reduce our problem to considering the vectors

$$F^n \operatorname{Re} l_k = \mathbb{H}^n c_k \otimes (\Omega h)^n \operatorname{Re} c_k \quad (4.2.20)$$

and

$$F^n \operatorname{Im} l_k = \mathbb{H}^n c_k \otimes (\Omega h)^n \operatorname{Im} c_k. \quad (4.2.21)$$

Another useful simplification is when the vectors $\operatorname{Re} c_k$ and $\operatorname{Im} c_k$ span \mathbb{R}^2 for all k and $\det h_S$ and $\det h_I$ are non-zero. In this case the vectors $(\Omega_2 h_S)^{n-i} (\Omega_2 h_I)^i \operatorname{Re} c_k$ and $(\Omega_2 h_S)^{n-i} (\Omega_2 h_I)^i \operatorname{Im} c_k$ will always span \mathbb{R}^2 and we can reduce our problem to an N

dimensional case where we consider only the macro structure of the system. We took advantage of this in the previous example of a chain N of harmonic oscillators with a heat bath environment. Note however that if we took a scattering environment, as we did in (3.4.3), then this is not the case as $\text{span}\{\text{Re } l_k\} = \mathbb{R}$ and this led to the situation where we had subspaces V_j which were given by superpositions of degrees of freedom in different subsystems, as opposed to superpositions of the subsystems themselves.

4.3 Further simple examples

4.3.1 A Loop

Now let's look at another obvious simple case, that of a ring or loop of harmonic oscillators with the same internal Hamiltonian and the same interaction, in particular, all internal harmonic oscillator frequencies ω are the same and all interaction frequencies δ are the same. As before we will consider a heat bath environment coupled to one oscillator.

We begin by considering the 3 oscillator case, note that due to the symmetry of the system, which particle we couple to is irrelevant. This is shown diagrammatically in Fig. 4.5.

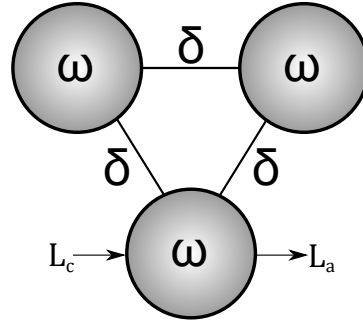


Figure 4.5: A loop of 3 harmonic oscillators with the same frequency ω and interaction δ . The heat bath coupling is indicated by a creation operator pumping information into the system and an annihilation operator pumping energy out of the system.

In this case, we are in a situation where h_s and h_I are the same and using the simplification we highlighted above and we can diagonalize the matrix \mathbb{H} and use the same method that we used for the case of a chain of harmonic oscillators. The matrix \mathbb{H} is given by

$$\mathbb{H} = \begin{pmatrix} \omega & \delta & \delta \\ \delta & \omega & \delta \\ \delta & \delta & \omega \end{pmatrix} \quad (4.3.1)$$

which is in the form of a *Circulant Matrix*. That is, each row is a right cyclic shift of the

row above it. More precisely, a circulant matrix is a matrix of the following form [15]:

$$C_n = \begin{pmatrix} c_0 & c_1 & c_2 & \cdots & c_{n-1} \\ c_{n-1} & c_0 & c_1 & c_2 & \vdots \\ & c_{n-1} & c_0 & c_1 & \ddots \\ \vdots & \ddots & \ddots & \ddots & c_2 \\ c_1 & \cdots & & c_{n-1} & c_0 \end{pmatrix}. \quad (4.3.2)$$

These matrices are particularly nice because the eigenvalues and eigenvectors, which we are ultimately interested in, are well known. In particular, they are given exactly by

$$\lambda_m = \sum_{k=0}^{n-1} c_k e^{\frac{-2\pi i m k}{n}} = \sum_{k=0}^{n-1} c_k \sigma_m^k \quad (4.3.3)$$

with associated eigenvector

$$\mathbf{v}_m = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 \\ \sigma_m \\ \sigma_m^2 \\ \vdots \\ \sigma_m^{n-1} \end{pmatrix} \quad (4.3.4)$$

where we have defined $\sigma_m = e^{\frac{-2\pi i m}{n}}$ as the n th roots of unity.

Using this, we have for the eigenvalues and eigenvectors of \mathbb{H} :

$$\lambda_1 = \omega + \delta\sigma_1 + \delta\sigma_1^2, \quad \mathbf{v}_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \sigma_1 \\ \sigma_1^2 \end{pmatrix}, \quad (4.3.5)$$

$$\lambda_2 = \omega + \delta\sigma_2 + \delta\sigma_2^2, \quad \mathbf{v}_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \sigma_2 \\ \sigma_2^2 \end{pmatrix}, \quad (4.3.6)$$

$$\lambda_3 = \omega + \delta\sigma_3 + \delta\sigma_3^2, \quad \mathbf{v}_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ \sigma_3 \\ \sigma_3^2 \end{pmatrix}. \quad (4.3.7)$$

Note two things then, first, that the matrix P constructed with the eigenvectors as its columns as above, is a unitary matrix. Hence its inverse is merely the Hermitian conjugate $P^{-1} = P^\dagger$ and hence it has no elements that are zero. This means that there are no single particle choices of the coupling vector \mathfrak{c} that will result in the first part of the determinant condition (4.1.67) being zero. What about the Vandermonde part? If we expand out our eigenvalues we find that

$$\lambda_1 = \omega + \delta\sigma_1 + \delta\sigma_1^2 = \omega - \delta, \quad (4.3.8)$$

$$\lambda_2 = \omega + \delta\sigma_2 + \delta\sigma_2^2 = \omega - \delta, \quad (4.3.9)$$

$$\lambda_3 = \omega + \delta\sigma_3 + \delta\sigma_3^2 = \omega + 2\delta. \quad (4.3.10)$$

Hence, $\lambda_1 = \lambda_2$ and as a result the Vandermonde determinant is zero. This means that, in the case of a 3 particle loop, for *any* single oscillator choice of environment coupling, the Hörmander condition will always fail.

Indeed, if as before we compute the orthogonal subspaces W_i in the 3 oscillator case and couple the heat bath to the first oscillator, we find

$$W_0 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right\} \otimes \mathbb{R}^2, \quad W_1 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} \right\} \otimes \mathbb{R}^2, \quad W_{df} = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.11)$$

and the evolution of the crossterms of a cat state centred in these subspaces is shown in Fig. 4.6.

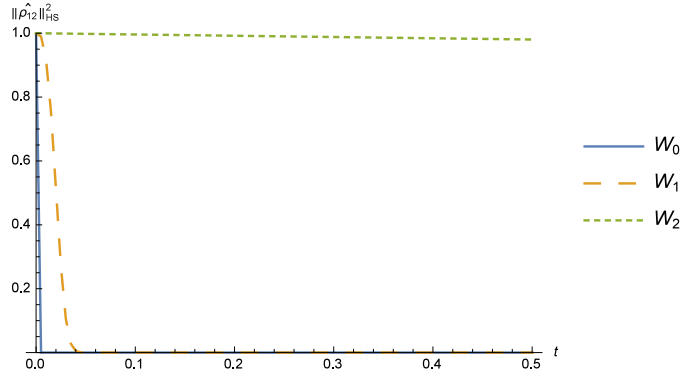


Figure 4.6: The Hilbert-Schmidt norm of $\rho_{12}(t, x)$ in Lemma 3.2.6 for a loop of three Harmonic oscillators and a heat bath environment coupled to the first oscillator initialised in the subspaces W_0, W_1 and $W_2 = W_{df}$ for $\hbar = 10^{-5}$, $\omega = 1$, $\delta = 1$, $\mu = 0.1$, $\gamma = 0.05$. Note that timelag in the onset of the decoherence and that the decoherence free subspace does not decay.

What about in the N oscillator loop case? We have the following result from Tee [24] which we quote verbatim:

Theorem 4.3.1 (Eigenvalues of circulant matrices [24]). *Every complex, symmetric circulant matrix of order N has a single eigenvalue with odd multiplicity if N is odd, but it has either two eigenvalues or none with odd multiplicity if N is even. All other eigenvalues occur with even multiplicity.*

In tabular form we have then

$$\begin{aligned} n \text{ odd} &\implies 1 \text{ odd multiplicity, rest even} \\ n \text{ even} &\implies 2 \text{ odd multiplicity, rest even} \\ &\text{OR all even.} \end{aligned}$$

Importantly for us then, apart from the cases of $N = 1$ and $N = 2$ (which don't really count as loops anyway), there are no possible situations in which the matrix \mathbb{H} for a loop of harmonic oscillators doesn't have at least one repeated eigenvalue (even multiplicity). Thus we can state the following:

Remark 4.3.2. For single oscillator environment coupling, a loop of identical harmonic oscillators with identical nearest neighbour interactions will always fail the Hörmander condition. This means there is some protected subspace which will not experience decoherence.

4.3.2 A Star

We now consider another obvious configuration of harmonic oscillators and heat bath environment, namely a 'star' where one oscillator is connected to all others and no others are connected. Lets consider the simplest possible case of this that hasn't already been covered, namely the case where we have 4 oscillators, since 3 is just a line, shown in Fig. 4.7.

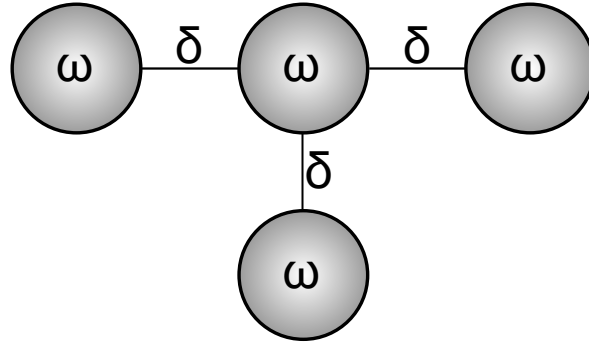


Figure 4.7: A 'star' of 4 harmonic oscillators with the same frequency ω and interaction δ .

Then we have that the matrix \mathbb{H} is given by

$$\mathbb{H} = \begin{pmatrix} \omega & \delta & \delta & \delta \\ \delta & \omega & 0 & 0 \\ \delta & 0 & \omega & 0 \\ \delta & 0 & 0 & \omega \end{pmatrix}. \quad (4.3.12)$$

There are only two distinct choices of oscillators we can couple the environment to, namely the central oscillator or one of the spokes. Let's begin by coupling to the central oscillator, then

$$W_0 = V_0 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \right\} \quad (4.3.13)$$

and hence immediately we see that

$$FV_0 = \text{span} \left\{ \begin{pmatrix} \omega \\ \delta \\ \delta \\ \delta \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.14)$$

and thus

$$W_1 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \right\} \otimes \mathbb{R}^2. \quad (4.3.15)$$

Hence, $V_1 \cong \mathbb{R}^4$. However now, if we take

$$FW_1 = \text{span} \left\{ \begin{pmatrix} 3\delta \\ \omega \\ \omega \\ \omega \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.16)$$

we see that

$$\begin{pmatrix} 3\delta \\ \omega \\ \omega \\ \omega \end{pmatrix} = 3\delta \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} + \omega \begin{pmatrix} 0 \\ 1 \\ 1 \\ 1 \end{pmatrix} \quad (4.3.17)$$

and hence $W_2 = \{0\}$. So by coupling the heat bath environment to the central oscillator, we can only reach a 4-dimensional subspace of the 8 dimensional phase space.

Note that this argument would proceed identically if we had a star consisting of N oscillators coupled to a central oscillator which was also coupled to the environment. At the first step we would obtain W_1 as the span of vectors

$$\begin{pmatrix} 0 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \otimes \mathbf{e}_{1,2} \quad (4.3.18)$$

and hence at the next step we would find $W_2 = \{0\}$.

Let us consider the other case then, when we couple to one of the outer oscillators. In this case,

$$W_0 = V_0 = \text{span} \left\{ \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.19)$$

and hence

$$FV_0 = \text{span} \left\{ \begin{pmatrix} \delta \\ \omega \\ 0 \\ 0 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.20)$$

and thus

$$W_1 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \right\} \otimes \mathbb{R}^2. \quad (4.3.21)$$

Now we are almost in the exact same situation as the previous case, if we compute

$$FW_1 = \text{span} \left\{ \begin{pmatrix} \omega \\ \delta \\ \delta \\ \delta \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.22)$$

we see straight away that

$$W_2 = \text{span} \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.23)$$

and by the same argument as before $W_3 = \{0\}$. Hence we made it one step further, and indeed we have a 6 dimensional subspace that is affected by decoherence, but there is still a 2 dimensional subspace

$$W_{df} = \text{span} \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.24)$$

which is decoherence free. Hence, a superposition of coherent states with centres $X_i = (0, 0, x_i, -x_i)$ will be protected from the onset of decoherence. Note again that this argument generalises to an N dimensional star directly, since

$$W_1 = \text{span} \left\{ \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.25)$$

and then

$$W_2 = \text{span} \left\{ \begin{pmatrix} 0 \\ 0 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \right\} \otimes \mathbb{R}^2 \quad (4.3.26)$$

and then $W_3 = \{0\}$ again.

So we can see that in this star setup, at best we can reach a 6 dimensional subspace of the system, irrespective of the number of oscillators coupled to the central oscillator, and indeed if we couple to the central oscillator the best we can do is a 4 dimensional subspace.

4.4 Outlook

In this chapter we looked at a set of basic example systems for which we could easily investigate how changing the macro structure of the system would affect the spread of decoherence induced at one oscillator. We used the motivating example of a chain of connected harmonic oscillators to determine a more general result for systems with linear Lindblad operators and quadratic Hamiltonians described by connected subsystems. In particular, we saw that by assuming a nice form of the interactions and environment we could simplify the problem massively to just investigating the linear independence of the N dimensional vectors $\mathbb{H}^j \mathbb{c}$. We used this simplification to investigate the chain of N oscillators, as well as the other simple cases of a loop and a star of N oscillators. Interestingly, we saw that for both the loop and the star, there was always a subspace protected from the influence of decoherence, given in terms of superpositions of states on the individual oscillators. For the chain it was not quite so simple, but we saw that if $N + 1$ was non-prime, then there was always some choice of environment coupling we could choose for which there would be a protected subspace.

These examples are all rather simplistic, but they server to highlight the advantages of the method, potentially provide building blocks from which more complicated systems can be constructed and possibly give some insight into the underlying properties of these graphs of connected oscillators that influence the spread of decoherence.

Further work in this area could be focussed in a few directions. Firstly, it might be possible to use the results for the chain, loop, and star to construct more complicated systems, and by knowing how decoherence spreads through these simple systems, determine how it spreads through the combined system.

Another direction would be to begin investigating more realistic systems where all subsystems are weakly coupled to the environment. In this case we would expect full decoherence as the space V_0 would immediately span \mathbb{R}^{2N} , but we could consider the situation where one subsystem is much more strongly coupled to the environment than the rest. In this situation we we would still expect full decoherence, but for short times we should see the effect of decoherence from the strongly coupled subsystem dominate and the same sort of timescales arising. We should also see 'weakly protected' subspaces which do not feel the decoherence from the strong coupling, but over time will still decohere from the weak coupling. From here we could possibly use this method to model a real world example of decoherence in a molecule.

Finally, it might be possible to give a more complete description of the symmetries and structure that leads to protected subspaces arising in these connected systems.

Chapter 5

A non-Hermitian Hamiltonian approach to the Lindblad equation

In this chapter we will present work which was published in the paper [12]. The focus of this paper was on the semiclassical evolution of the Wigner function of Gaussian states under the influence of the Lindblad equation. This was joint work with collaborators, so while we will discuss most of the points in the paper, we will primarily focus on the section to which we had the most input, namely the interpretation of the Lindblad equation as a non-Hermitian Schrödinger equation on a doubled phase space and the resulting evolution.

We will begin by motivating the use of this theory by placing it in context of the previous studies we made of the spread of decoherence. From here we will discuss the raising to a doubled phase space and the form of the non-Hermitian Hamiltonian that arises from this, before reviewing the previous results for the evolution of non-Hermitian Schrödinger equations. Finally we will relate these results back to previous results by Brodier and Ozorio de Almeida [3] as well as the other main results determined in [12].

5.1 Motivation: beyond linear Lindblads and quadratic Hamiltonians

In the previous chapters we determined results describing the extent and timescales of the spread of decoherence through a quantum system coupled to the environment. Importantly, the results we found were exact and this relied heavily on two specific assumptions we made, namely that Hamiltonian, given as the Weyl quantization of the symbol $H(x)$, was at most quadratic in x , and that the Lindblad operators, similarly given as the Weyl quantization of the symbols $L_k(x)$, were at most linear in x . As we saw in Section 2.2.5, while on the surface these restrictions seem quite strong, they actually cover a very large class of important systems, and in particular, as discussed in the previous chapter the harmonic oscillator heat bath model.

Nevertheless, we would like to extend our results beyond this quadratic Hamiltonian and linear Lindblad restriction to a wider class of system environment pairs. To this end we need a new method of dealing with the Lindblad equation on phase space. The key

element of the proof of Theorem 3.2.1 was the fact that the Lindblad equation became exact in the case of linear Lindblads and quadratic Hamiltonians, which meant we could reduce it to the form (2.6.28). Without this simplification, we are back in the general situation of the Lindblad equation on phase space as described in (2.6.4):

$$i\hbar \frac{\partial \rho}{\partial t} = H \star \rho - \rho \star H + i \sum_j L_j \star \rho \star \bar{L}_j - \frac{1}{2} \bar{L}_j \star L_j \star \rho - \frac{1}{2} \rho \star \bar{L}_j \star L_j. \quad (5.1.1)$$

Finding a general solution in the same way as before is no longer plausible, hence we need a new approach. To this end we will follow the ideas of [3] and reinterpret the phase space Lindblad equation as a Schrödinger equation on a doubled phase space.

5.2 Interpreting the Lindblad equation as a Schrödinger equation

In this section we will introduce the method used in section 4 of [12] which allows us to lift the Lindblad equation to a Schrödinger equation on doubled phase space.

We start by mentioning that Brodier and Ozorio de Almeida in [3] introduced this idea of the doubled phase space to derive an approximate Gaussian solution to the Lindblad equation in the semiclassical limit in the case of a *general* Hamiltonian but still restricted to linear Lindblads. We intend to be more general still by allowing for arbitrary Lindblad operators. Later we will compare the methods and results of the two approaches.

Our starting point is the general Lindblad equation on phase space we recalled above (5.1.1). Here however, instead of using ρ (or equivalently W) for our Wigner function, we will instead use ψ to indicate that we should be thinking of this as the evolution of a wave-function. Recall then that we have

$$i\hbar \frac{\partial \psi}{\partial t} = H \star \psi - \psi \star H + i \sum_j L_j \star \psi \star \bar{L}_j - \frac{1}{2} \bar{L}_j \star L_j \star \psi - \frac{1}{2} \psi \star \bar{L}_j \star L_j. \quad (5.2.1)$$

Here we had intentionally rearranged so that we had a LHS of the form $i\hbar \frac{\partial \psi}{\partial t}$ in keeping with the standard way of writing the Schrödinger equation. It is not difficult then to imagine that we could rewrite (5.2.1) as

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}}(\hat{x}, \hat{y}) \psi. \quad (5.2.2)$$

Here we are taking our $\hat{x} = (q, p)$ and our $\hat{y} = (-i\hbar \nabla_q, -i\hbar \nabla_p)$ as our position and 'momentum' variables on a *doubled phase space* and we are defining $\hat{\mathcal{H}}(\hat{x}, \hat{y})$ as our Hamiltonian on our doubled phase space. Note that the pair of operators \hat{x} and \hat{y} as defined above are Hermitian operators and importantly satisfy the canonical commutation relations

$$[\hat{x}_i, \hat{y}_j] = i\hbar \delta_{ij} \quad (5.2.3)$$

and

$$[\hat{x}_i, \hat{x}_j] = 0, \quad [\hat{y}_i, \hat{y}_j] = 0. \quad (5.2.4)$$

Hence it is valid to treat these operators as position and momentum operators on this doubled phase space.

Lets determine the form of the Hamiltonian $\hat{\mathcal{H}}$. We start by introducing the following result (this is discussed in e.g. [27] which considers a similar idea for the von-Neumann equation) that allows us to interpret the Moyal product $a \star b$ as the application of an operator on our phase space function ψ .

Lemma 5.2.1 (Moyal product as an operator). *Suppose we have two phase space functions $A(x)$ and $\psi(x)$ then we have the following results for the Moyal product:*

$$A \star \psi = \hat{A}^{(-)}\psi \quad \text{and} \quad \psi \star A = \hat{A}^{(+)}\psi, \quad (5.2.5)$$

where

$$\hat{A}^{(\pm)} = A(\hat{x} \pm \frac{1}{2}\Omega\hat{y}) \quad (5.2.6)$$

is an operator acting on the phase space function $\psi(x)$ with

$$\hat{x} = (q, p) \quad (5.2.7)$$

$$\hat{y} = (-i\hbar\nabla_q, -i\hbar\nabla_p) \quad (5.2.8)$$

as before.

Proof. Our starting point is the integral representation of $a \star b$ (2.5.46):

$$A \star \psi(x) = \frac{1}{(\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{2i}{\hbar}w_1 \cdot \Omega w_2} A(x + w_1) \psi(x + w_2) dw_1 dw_2 \quad (5.2.9)$$

for $x = (q, p)$. The aim is to rewrite this in the form

$$A \star \psi(x) = \int_{\mathbb{R}^{2n}} K(x, w_2) \psi(w_2) dw_2 \quad (5.2.10)$$

where $K(x, w_2)$ is an integral kernel and in particular, we wish $K(x, w_2)$ to be the Weyl quantization of some symbol.

We start by making the substitution $w_2 \rightarrow w_2 - x$. Then we have, with some rearranging

$$A \star \psi(x) = \int_{\mathbb{R}^{2n}} \frac{1}{(\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{-\frac{2i}{\hbar}w_1 \cdot \Omega^T(w_2 - x)} A(x + w_1) dw_1 \psi(w_2) dw_2. \quad (5.2.11)$$

Now we make the substitution $w_1 \rightarrow \frac{1}{2}w_1$, which gives

$$A \star \psi(x) = \int_{\mathbb{R}^{2n}} \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar}w_1 \cdot \Omega^T(x - w_2)} A(x + \frac{1}{2}w_1) dw_1 \psi(w_2) dw_2 \quad (5.2.12)$$

and we can identify our integral kernel as

$$K(x, w_2) = \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar}w_1 \cdot \Omega^T(x - w_2)} A(x + \frac{1}{2}w_1) dw_1. \quad (5.2.13)$$

5.2. INTERPRETING THE LINDBLAD EQUATION AS A SCHRÖDINGER EQUATION

Now we make the substitution $w_1 \rightarrow w_1 - 2s(x - w_2)$. Note that this only affects the argument of a since

$$-2s(x - w_2) \cdot \Omega^T(x - w_2) = 0, \quad \forall s. \quad (5.2.14)$$

Hence we have

$$K(x, w_2) = \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} w_1 \cdot \Omega^T(x - w_2)} A(x - s(x - w_2) + \frac{1}{2}w_1) dw_1 \quad (5.2.15)$$

and upon making the substitution $y = -\Omega^T w_1$ we find

$$K(x, w_2) = \frac{1}{(2\pi\hbar)^{2n}} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar} y \cdot (x - w_2)} A((1 - s)x + sw_2 - \frac{1}{2}\Omega y) dy. \quad (5.2.16)$$

If we compare this with (2.5.14) we see, taking $t = (1 - s)$, that this is just the integral kernel of the quantization $\text{Op}_t(A^{(-)})b(x)$ where

$$A^{(-)}(x) := A(x - \frac{1}{2}\Omega y). \quad (5.2.17)$$

This gives the first result, for the second note that the exact same method holds if we invert the order of A and ψ , it is merely the sign of Ω that changes in the exponential. Note that this result holds for any quantization, i.e. for any $t \in [0, 1]$ and not just the Weyl quantization. \square

Using this lemma we can directly translate our Lindblad equation (5.2.1) into the Schrödinger equation (5.2.2).

Theorem 5.2.2. *We can write the Lindblad equation on phase space (5.2.1) in the form of a Schrödinger equation*

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}}(\hat{x}, \hat{y}) \psi. \quad (5.2.18)$$

where the Hamiltonian is given by

$$\hat{\mathcal{H}}(\hat{x}, \hat{y}) = \hat{H}^{(-)} - \hat{H}^{(+)} + i \sum_k \hat{L}_k^{(-)} \hat{\bar{L}}_k^{(+)} - \frac{1}{2} \left(\widehat{\bar{L}_k \star L_k} \right)^{(+)} - \frac{1}{2} \left(\widehat{\bar{L}_k \star L_k} \right)^{(-)}. \quad (5.2.19)$$

Proof. This is a direct application of Lemma 5.2.1. Starting from

$$i\hbar \frac{\partial \psi}{\partial t} = H \star \psi - \psi \star H + i \sum_j L_j \star \psi \star \bar{L}_j - \frac{1}{2} \bar{L}_j \star L_j \star \psi - \frac{1}{2} \psi \star \bar{L}_j \star L_j \quad (5.2.20)$$

and applying it to each term in the expansion. \square

Note in particular that this Hamiltonian is manifestly *non-Hermitian* and, assuming a Hermitian choice of the internal Hamiltonian H , the non-Hermitian part arises from the interaction with the environment described by the Lindblad operators. This is perhaps to be expected since non-Hermitian Hamiltonians have long been used to describe open quantum systems [36].

Given this operator form of the Hamiltonian, we can then directly apply the Wigner-Weyl transform to arrive at the following associated double-phase space function:

$$\mathcal{H} = H^{(-)} - H^{(+)} + i \sum_k L_k^{(-)} \star_2 \bar{L}_k^{(+)} - \frac{1}{2} (\bar{L}_k \star L_k)^{(+)} - \frac{1}{2} (\bar{L}_k \star L_k)^{(-)} \quad (5.2.21)$$

or explicitly

$$\begin{aligned} \mathcal{H}(x, y) = & H\left(x - \frac{1}{2}\Omega y\right) - H\left(x + \frac{1}{2}\Omega y\right) + i \sum_k L_k\left(x - \frac{1}{2}\Omega y\right) \star_2 \bar{L}_k\left(x + \frac{1}{2}\Omega y\right) \\ & - \frac{1}{2} (\bar{L}_k \star L_k)\left(x + \frac{1}{2}\Omega y\right) - \frac{1}{2} (\bar{L}_k \star L_k)\left(x - \frac{1}{2}\Omega y\right). \end{aligned} \quad (5.2.22)$$

Here we have used \star_2 to denote the star product on the doubled phase space, defined analogously to the normal star product (2.5.44).

Proposition 5.2.3. *Assuming that \hat{H} and \hat{L}_k are quantizations of \hbar independent symbol functions H and L_k . Then, semiclassically expanding $\mathcal{H}(x, y)$ we have the following expansion to first order in \hbar :*

$$\mathcal{H} = \mathcal{H}^{(0)} + \hbar \mathcal{H}^{(1)} + O(\hbar^2) \quad (5.2.23)$$

where

$$\mathcal{H}^{(0)} = H^{(-)} - H^{(+)} + \sum_k \text{Im}(\bar{L}_k^{(-)} L_k^{(+)}) - \frac{i}{2} \sum_k |L_k^{(+)} - L_k^{(-)}|^2, \quad (5.2.24)$$

which is a separation into real and imaginary parts, and

$$\mathcal{H}^{(1)} = \frac{1}{2} \sum_k \{\bar{L}_k, L_k\}^{(+)} + \{\bar{L}_k, L_k\}^{(-)} \quad (5.2.25)$$

which is purely imaginary.

Proof. Since we assume H and L_k are \hbar independent, we only have to compute the star product expansions. Starting with the term $L_k^{(-)} \star_2 \bar{L}_k^{(+)}$ we have

$$L_k^{(-)} \star_2 \bar{L}_k^{(+)} = L_k^{(-)} \bar{L}_k^{(+)} + \frac{i\hbar}{2} \{L_k^{(-)}, \bar{L}_k^{(+)}\} + O(\hbar^2) \quad (5.2.26)$$

where the Poisson bracket is the Poisson bracket on *doubled* phase space. Similarly,

$$\bar{L}_k \star L_k = \bar{L}_k L_k + \frac{i\hbar}{2} \{\bar{L}_k, L_k\} + O(\hbar^2). \quad (5.2.27)$$

Hence, collecting terms, we have

$$\mathcal{H}^{(0)} = H^{(-)} - H^{(+)} + i \sum_k L_k^{(-)} \bar{L}_k^{(+)} - \frac{1}{2} \left((\bar{L}_k L_k)^{(+)} + (\bar{L}_k L_k)^{(-)} \right), \quad (5.2.28)$$

and

$$\mathcal{H}^{(1)} = \frac{1}{2} \sum_k \{ \bar{L}_k, L_k \}^{(+)} + \{ \bar{L}_k, L_k \}^{(-)} - \{ L_k^{(-)}, \bar{L}_k^{(+)} \}. \quad (5.2.29)$$

Focussing first on $\mathcal{H}^{(0)}$, we expand $(\bar{L}_k L_k)^{(\pm)} = \bar{L}_k^{(\pm)} L_k^{(\pm)}$ and then write

$$L_k^{(-)} \bar{L}_k^{(+)} = \operatorname{Re} \left(L_k^{(-)} \bar{L}_k^{(+)} \right) + i \operatorname{Im} \left(L_k^{(-)} \bar{L}_k^{(+)} \right). \quad (5.2.30)$$

Then, using

$$\operatorname{Re} \left(L_k^{(-)} \bar{L}_k^{(+)} \right) = \frac{1}{2} \left(L_k^{(-)} \bar{L}_k^{(+)} + \bar{L}_k^{(-)} L_k^{(+)} \right) \quad (5.2.31)$$

we see that all the remaining terms in the sum can be written as

$$\begin{aligned} & i \sum_k L_k^{(-)} \bar{L}_k^{(+)} - \frac{1}{2} \left((\bar{L}_k L_k)^{(-)} + (\bar{L}_k L_k)^{(+)} \right) \\ &= i \sum_k i \operatorname{Im} \left(L_k^{(-)} \bar{L}_k^{(+)} \right) - \frac{1}{2} \left(\bar{L}_k^{(+)} L_k^{(+)} + \bar{L}_k^{(-)} L_k^{(-)} - L_k^{(-)} \bar{L}_k^{(+)} - \bar{L}_k^{(-)} L_k^{(+)} \right) \\ &= \sum_k \operatorname{Im} \left(\bar{L}_k^{(-)} L_k^{(+)} \right) - \frac{i}{2} \sum_k |L_k^{(+)} - L_k^{(-)}|^2 \end{aligned} \quad (5.2.32)$$

and hence

$$\mathcal{H}^{(0)} = H^{(-)} - H^{(+)} + \sum_k \operatorname{Im} \left(\bar{L}_k^{(-)} L_k^{(+)} \right) - \frac{i}{2} \sum_k |L_k^{(+)} - L_k^{(-)}|^2, \quad (5.2.33)$$

as given.

Now we focus on the second term, $\mathcal{H}^{(1)}$. Here we need to show that the term $\{ L_k^{(-)}, \bar{L}_k^{(+)} \}$ is zero. If we find this directly we have that

$$\{ L_k^{(-)}, \bar{L}_k^{(+)} \} = \frac{\partial L_k^{(-)}}{\partial x_i} \frac{\partial \bar{L}_k^{(+)}}{\partial y_i} - \frac{\partial L_k^{(-)}}{\partial y_i} \frac{\partial \bar{L}_k^{(+)}}{\partial x_i} \quad (5.2.34)$$

and computing

$$\frac{\partial L_k}{\partial y_i} (x \pm \frac{1}{2} \Omega y) = \frac{\partial L_k}{\partial x_j} \frac{\partial (\pm \frac{1}{2} \Omega y)_j}{\partial y_i} \quad (5.2.35)$$

we see that

$$\frac{\partial (\pm \frac{1}{2} \Omega y)_j}{\partial y_i} = \partial_{y_i} (\pm \frac{1}{2} \Omega_{jk} y_k) = \pm \frac{1}{2} \Omega_{jk} \delta_{ki} = \pm \frac{1}{2} \Omega_{ji}. \quad (5.2.36)$$

Hence,

$$\frac{\partial L_k}{\partial y_i} (x \pm \frac{1}{2} \Omega y) = \pm \frac{1}{2} \Omega_{ji} \partial_{x_i} L_k (x \pm \frac{1}{2} \Omega y) = \left[\pm \frac{1}{2} \Omega^T \nabla_x L_k (x \pm \frac{1}{2} \Omega y) \right]_i. \quad (5.2.37)$$

Using this we see that

$$\begin{aligned}\{L_k^{(-)}, \bar{L}_k^{(+)}\} &= \frac{1}{2} (\nabla_x L_k \cdot \Omega^T \nabla_x \bar{L}_k + \Omega^T \nabla_x L_k \cdot \nabla_x \bar{L}_k) \\ &= \frac{1}{2} \nabla_x L_k \cdot (\Omega^T + \Omega) \nabla_x \bar{L}_k = 0.\end{aligned}\tag{5.2.38}$$

Finally then, we just have to show that the remaining terms in $\mathcal{H}^{(1)}$ are purely imaginary, this is immediate since

$$\overline{\{\bar{L}_k, L_k\}} = \{L_k, \bar{L}_k\} = -\{\bar{L}_k, L_k\}\tag{5.2.39}$$

and hence $\text{Re } \mathcal{H}^{(1)} = 0$. \square

One should note here that although we have specified that H and L_k are \hbar independent, this is not a strict requirement and we could allow for more general functions that admit a semiclassical expansion in \hbar in the same vein as \mathcal{H} . In this case $\mathcal{H}^{(0)}$ would involve terms in $H^{(0)}$ and $L_k^{(0)}$, while $\mathcal{H}^{(1)}$ would be determined by terms in $H^{(0)}$, $L_k^{(0)}$ and $L_k^{(1)}$.

As mentioned, the Hamiltonian \mathcal{H} is a distinctly non-Hermitian Hamiltonian. There exists an emerging theory behind the evolution of Schrödinger equations with non-Hermitian Hamiltonians, in particular for Gaussian states, which we will review in the next section and then apply to the Hamiltonian \mathcal{H} we just determined.

5.3 Lindblad and the theory of non-Hermitian Hamiltonians

5.3.1 The theory of non-Hermitian Hamiltonians

In this section we will recall the recent work on the subject of non-Hermitian Hamiltonians in preparation for applying the theory to the Lindblad equation. In particular, we will review the work previously undertaken by co-authors R. Schubert and E.M. Graefe in two papers on Gaussian wave packet evolution in non-Hermitian systems. The first of these [13] was a short paper which extended the well known theory of Hepp [18] and Heller [17] (a good review of this as well as many other results in the area was given by Littlejohn [34]) on describing the motion of the centres of Gaussian states in the semiclassical limit. Importantly, this evolution is given by Hamilton's classical equations of motion in the case of closed quantum systems. By applying the same ideas to the non-Hermitian description of open systems they arrived at a modified set of evolution equations for the centre, covariance and phase of the Wigner function, which can be considered as, quoting [13], "the semiclassical limit of non-Hermitian quantum dynamics".

In the second paper [14] the underlying complex symplectic geometry of these equations and the evolution of complexified coherent states under non-Hermitian Hamiltonians is investigated. In particular, a class of coherent states with formally complex centres in phase space is considered and a set of equations for the centre, width and phase of

the Wigner function are again determined. It is then shown that these equations can be projected onto the equations describing the evolution of the real counterparts via a complex structure J (see Section 2.3.4 for an overview of complex structures) which is further investigated. While this underlying complex structure is very interesting, for our purposes we will not need these complexified coherent states and as a result we will focus our attention on reviewing the main results of [13].

Our starting point is the non-Hermitian Wigner von-Neumann equation which we decompose into the Hermitian and non-Hermitian parts as follows:

$$i\hbar \frac{\partial \hat{W}}{\partial t} = [\hat{H}, \hat{W}] - i [\hat{\Gamma}, \hat{W}]_+ . \quad (5.3.1)$$

Here we consider \hat{H} and $\hat{\Gamma}$ to be given by the Weyl quantization of sufficiently nice classical observables H and Γ respectively. As usual the notation $[\cdot, \cdot]$ represents the commutator and we are using the notation $[\cdot, \cdot]_+$ to represent the anti-commutator.

We will consider this equation for the evolution of Gaussian states of the form $\psi_Z^B(x)$ as described in (2.7.3) with associated Gaussian Wigner functions as $W(z)$ as described in (2.7.5) where, since we will later be applying this to a doubled phase space, we use the notation $z = (x, y)$.

The evolution of the Wigner function on phase space can then be readily determined as the following:

$$i\hbar \frac{\partial W}{\partial t} = H \star W - W \star H - i(\Gamma \star W + W \star \Gamma) . \quad (5.3.2)$$

Here \star represents the star product as described before (2.5.43). Now we use the semi-classical expansion (2.5.49) to arrive at the following expansion for the Hermitian part

$$H \star W - W \star H = i\hbar \{H, W\} + O(\hbar^3) \quad (5.3.3)$$

and similarly, if we consider the expansion of the non-Hermitian part we arrive at

$$\Gamma \star W + W \star \Gamma = 2\Gamma W - \frac{\hbar^2}{4} \Gamma \left(\overleftarrow{\nabla}_z \cdot \Omega \overrightarrow{\nabla}_z \right)^2 W + O(\hbar^4) . \quad (5.3.4)$$

The non-Hermitian part is a bit more complicated to work with but we can simplify it by rewriting the second term as

$$-\frac{\hbar^2}{4} \Gamma \left(\overleftarrow{\nabla}_z \cdot \Omega \overrightarrow{\nabla}_z \right)^2 W = -\frac{\hbar^2}{4} (\nabla_z \cdot \Omega^T \Gamma''(z) \Omega \nabla_z) W = -\frac{\hbar^2}{4} \Delta_\Gamma W \quad (5.3.5)$$

where we have defined $\Gamma''(z)$ to be the matrix of second derivatives of Γ at z . Note then that Δ_Γ is Hermitian and if $\Gamma''(z)$ is symplectic then $\Gamma''^{-1} = \Omega^T \Gamma'' \Omega$. Hence, as implied by the choice of notation, Δ_Γ is the Laplace-Beltrami operator defined by Γ'' .

Given the above expansions, to leading order in \hbar we can write our non-Hermitian Wigner von-Neumann equation as

$$\hbar \frac{\partial W}{\partial t} = - \left(-\frac{\hbar^2}{4} \Delta_\Gamma W - \hbar \nabla_z H \cdot \Omega \nabla_z + 2\Gamma \right) W. \quad (5.3.6)$$

where we have used the standard expansion of the Poisson bracket $\{a, b\} = \nabla a \cdot \Omega \nabla b$. Note that for the case of no Γ we return to the classical Liouville equation (as we would expect).

Now we make a Gaussian ansatz for the Wigner function

$$W(t, z) = \frac{\alpha(t)}{(\pi \hbar)^n} e^{\frac{i}{\hbar} \delta z \cdot G(t) \delta z}, \quad \delta z := z - Z(t). \quad (5.3.7)$$

Upon simply plugging this ansatz in to our evolution equation we arrive at

$$\left[\hbar \frac{\dot{\alpha}}{\alpha} + 2\dot{Z} \cdot G \delta z - \delta z \cdot \dot{G} \delta z \right] W(z) = \left[\delta z \cdot G \Omega^\Gamma \Gamma'' \Omega G \delta z - 2 \nabla H \cdot \Omega G \delta z - \frac{\hbar}{2} \text{tr}(\Gamma'' \Omega G \Omega^\Gamma) - 2\Gamma \right] W \quad (5.3.8)$$

Here we simply expand our symbols $\Gamma(z)$ and $H(z)$ up to second order around the point $z = Z$. Doing so we get

$$\Gamma(z) \approx \Gamma(Z) + \nabla \Gamma(Z) \cdot \delta z + \frac{1}{2} \delta z \cdot \Gamma''(Z) \delta z \quad (5.3.9)$$

$$\nabla H(z) \approx \nabla H(Z) + H''(Z) \delta z. \quad (5.3.10)$$

The remainder terms here are of $O(\hbar^{3/2})$. Plugging this in and separating powers of δz we arrive at the following set of equations:

$$(\delta z)^0 : \quad \frac{\dot{\alpha}}{\alpha} = -\frac{2}{\hbar} \Gamma(Z) - \frac{1}{2} \text{tr}(\Gamma''(Z) \Omega G \Omega^\Gamma) \quad (5.3.11)$$

where we have used the cyclic property of the trace.

$$(\delta z)^1 : \quad 2G^\Gamma \dot{Z} = -2G^\Gamma \Omega^\Gamma \nabla H(Z) - 2 \nabla \Gamma(Z) \quad (5.3.12)$$

which since G is symmetric and $\Omega^\Gamma = -\Omega$ gives us the equation

$$\dot{Z} = \Omega \nabla H(Z) - G^{-1} \Gamma(Z). \quad (5.3.13)$$

Finally, $(\delta z)^2$:

$$\dot{G} = H''(Z) \Omega G - G \Omega H''(Z) + \Gamma''(Z) - G \Omega^\Gamma \Gamma''(Z) \Omega G \quad (5.3.14)$$

where we have used the fact that only the symmetric part of G is important in $W(t, z)$ since it appears only in a quadratic form, hence we have enforced the convention $(G^\Gamma + G)/2 = G$.

After all this then, we arrive at the following set of equations which describe the evolution of the Wigner function of our Gaussian under the influence of a non-Hermitian Schrödinger equation:

Theorem 5.3.1 (Graefe-Schubert 2011 [13]). *For a Gaussian Wigner function of the form:*

$$W(t, z) = \frac{\alpha(t)}{(\pi\hbar)^n} e^{\frac{i}{\hbar} \delta z \cdot G(t) \delta z}, \quad \delta z := z - Z(t) \quad (5.3.15)$$

evolving under the influence of the non-Hermitian Schrödinger equation:

$$i\hbar \frac{\partial \hat{W}}{\partial t} = [\hat{H}, \hat{W}] - i [\hat{\Gamma}, \hat{W}]_+ \quad (5.3.16)$$

we have the following set of evolution equations for Z, G and α :

$$\dot{Z} = \Omega \nabla H(Z) - G^{-1} \Gamma(Z), \quad (5.3.17)$$

$$\dot{G} = H''(Z) \Omega G - G \Omega H''(Z) + \Gamma''(Z) - G \Omega^T \Gamma''(Z) \Omega G, \quad (5.3.18)$$

$$\frac{\dot{\alpha}}{\alpha} = -\frac{2}{\hbar} \Gamma(Z) - \frac{1}{2} \text{tr}(\Gamma''(Z) \Omega G \Omega^T). \quad (5.3.19)$$

By finding $Z(t)$ and $G(t)$ using this set of equations, one can determine the expectation of an arbitrary observable \hat{A} in the small \hbar regime in terms of the (smooth) symbol A via

$$\langle \hat{A} \rangle_W = A(Z) + O(\hbar) \quad (5.3.20)$$

and similarly the variance of A via

$$(\Delta \hat{A})_\psi^2 = \frac{\hbar}{2} \nabla A(Z) \cdot G^{-1} \nabla A(Z) + O(\hbar^2). \quad (5.3.21)$$

As discussed in [13] this non-Hermitian Hamiltonian $H - i\Gamma$ introduces dynamics in the classical limit which are not Hamiltonian, but rather consist of a Hamiltonian part and a gradient part. Further discussion of the equations (5.3.17-5.3.18) can be found in [13] and [14], importantly note the evolution equation for G (5.3.18) preserves the symplecticness of G .

To come to this set of equations we had to expand $H(z)$ and $\Gamma(z)$ around the point $z = Z(t)$, and we expect this expansion to be accurate as long as the Wigner function $W(t, z)$ is strongly localised around this centre $z = Z(t)$. Since the matrix $G(t)$ remains symplectic $\|G^{-1}\| = \|G\|$ and hence this can be guaranteed if

$$\hbar \|G\| \ll 1. \quad (5.3.22)$$

An equivalent approach is to take the state $\psi(t, x) = e^{i\alpha(t)} \psi_{z_c(t)}^{B(t)}(x)$ as a Gaussian ansatz for the Schrödinger equation where $z_c(t)$ is now a complex centre

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}} \psi \quad (5.3.23)$$

where, comparing to the above, $\mathcal{H} = H - i\Gamma$ and separating terms in powers of $(x - x_c(t))$, one can determine the following equations for $z_c(t)$, $B(t)$ and $\alpha(t)$:

$$-\dot{y}_c + B\dot{x}_c = \mathcal{H}_q + B\mathcal{H}_p, \quad (5.3.24)$$

$$\dot{B} = -B\mathcal{H}_{yy}B - B\mathcal{H}_{yx} - \mathcal{H}_{xy}B - \mathcal{H}_{xx}, \quad (5.3.25)$$

and

$$\dot{\alpha} = \frac{1}{\hbar}[y_c \cdot \dot{x}_c - \mathcal{H}] + \frac{i}{2}[\text{tr } \mathcal{H}_{pq} + \text{tr}(\mathcal{H}_{pp}B)] - \frac{i}{\hbar} \text{tr}(\dot{B}B^{-1}). \quad (5.3.26)$$

The two sets of equations are compatible if $x_c(t) = X(t)$ and $y_c(t) = Y(t)$ are demanded to be real. This compatibility and the deep symplectic structure behind this approach to the evolution of complexified coherent states are discussed in detail in [14] but for our purposes here we merely focus on the equivalence between the equation for G (5.3.18) and the comparatively simpler equation for B (5.3.25) which we will be preferred in what follows.

5.3.2 Schrödinger evolution of the Lindblad equation

Having put the Lindblad equation in a Schrödinger form (5.2.18) we are now in a position to determine the evolution of Gaussian states under the Lindblad equation.

Our starting point is the initial state

$$\psi_Z^B(x) = \frac{(\det B)^{1/4}}{(\pi\hbar)^{n/2}} e^{\frac{i}{\hbar}[\frac{1}{2}(x-X) \cdot B(x-X) + Y \cdot (x-X) + \alpha]} \quad (5.3.27)$$

where $Z = (X, Y) \in \mathbb{R}^{4n}$ and $\alpha \in \mathbb{C}$ is a phase factor. This Gaussian with a linear term is the kind of state that appears when finding the Wigner function of a superposition of Gaussian states (see Section 2.7.3) and allows our theory to apply to general initial states.

In particular, given this form, we can now directly apply the equations derived in [13] and recalled in Theorem 5.3.1 with the non-Hermitian Hamiltonian determined above to arrive at the following set of evolution equations for Z, B and α :

Theorem 5.3.2. *For an initial state on doubled phase space given by*

$$\psi_Z^B(x) = \frac{(\det B)^{1/4}}{(\pi\hbar)^{n/2}} e^{\frac{i}{\hbar}[\frac{1}{2}(x-X) \cdot B(x-X) + Y \cdot (x-X) + \alpha]} \quad (5.3.28)$$

$Z = (X, Y)$, $\text{Im } B > 0$, evolving under the doubled phase space Schrödinger equation:

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{\mathcal{H}}(\hat{x}, \hat{y}) \psi(x, t) \quad (5.3.29)$$

where

$$\hat{\mathcal{H}}(\hat{x}, \hat{y}) = \hat{H}^{(-)} - \hat{H}^{(+)} + i \sum_k \hat{L}_k^{(-)} \hat{L}_k^{(+)} - \frac{1}{2} \left(\widehat{\bar{L}_k \star L_k} \right)^{(+)} - \frac{1}{2} \left(\widehat{\bar{L}_k \star L_k} \right)^{(-)}. \quad (5.3.30)$$

we have the following set of equations describing the evolution of Z, B and α in the semiclassical limit:

$$\dot{Z} = \Omega_2 \nabla \operatorname{Re} \mathcal{H}^{(0)} + \mathcal{G}^{-1} \nabla \operatorname{Im} \mathcal{H}^{(0)}, \quad (5.3.31)$$

$$\dot{B} = -B \mathcal{H}_{yy}^{(0)} B - B \mathcal{H}_{yx}^{(0)} - \mathcal{H}_{xy}^{(0)} B - \mathcal{H}_{xx}^{(0)}, \quad (5.3.32)$$

$$\dot{\alpha} = \frac{i\hbar}{4} \operatorname{tr} \left(\dot{B} B^{-1} \right) + Y \cdot \dot{X} - \mathcal{H}^{(0)}(X, Y) - \hbar \mathcal{H}^{(1)}(X, Y) \quad (5.3.33)$$

$$+ \frac{i\hbar}{2} \operatorname{tr} \left(\mathcal{H}_{xy}^{(0)} + \mathcal{H}_{yy}^{(0)} B \right). \quad (5.3.34)$$

Here we have taken $\nabla := (\partial_x, \partial_y)$ as the doubled phase space gradient, Ω_2 as the doubled phase space symplectic form and

$$\mathcal{H}_{xy} := (\partial_{x_i} \partial_{y_j} \mathcal{H})$$

which notably satisfies $\mathcal{H}_{yx} = (\mathcal{H}_{xy})^T$.

The matrix \mathcal{G} is given by

$$\mathcal{G} = \begin{pmatrix} \operatorname{Im} B + \operatorname{Re} B [\operatorname{Im} B]^{-1} \operatorname{Re} B & -\operatorname{Re} B [\operatorname{Im} B]^{-1} \\ -[\operatorname{Im} B]^{-1} \operatorname{Re} B & [\operatorname{Im} B]^{-1} \end{pmatrix}. \quad (5.3.35)$$

Proof. The equation for Z follows directly from applying (5.3.17) to the first term in the expansion (5.2.23). Similarly, the equation for the evolution of B follows from (5.3.25) or an equivalent equation for \mathcal{G} which would follow from (5.3.18).

Finally, the equation for α follows from (5.3.26) though here it should be noted that the term $\mathcal{H}^{(1)}$ is also needed in the expansion (see for instance section 3.5 of [46]). \square

Lets give an example of using the result for the doubled phase space method to investigate the interference terms of a cat state initial Wigner function evolving under a damped anharmonic oscillator. This is the same example as produced in [12].

Example 5.3.3. We consider the anharmonic oscillator described by internal Hamiltonian

$$\hat{H} = \frac{1}{2}(\hat{q}^2 + \hat{p}^2) + \frac{\beta}{4}\hat{q}^4 \quad (5.3.36)$$

where we have taken natural units with $\hbar = m = \omega = 1$. The variable β here determines the degree of anharmonicity. For our Lindblad operator we choose a single annihilation operator

$$\hat{L} = \sqrt{\frac{\gamma}{2}}(\hat{q} + i\hat{p}) \quad (5.3.37)$$

where the variable γ describes the degree of damping. For $\beta = 0$, we have exact results since are in the situation of a quadratic Hamiltonian and linear Lindblad operator that we have already studied in great detail in the previous chapters.

If we find the symbol $\mathcal{H}(x, y)$ we find

$$\mathcal{H}^{(0)}(x, y) = (\Omega x) \cdot y - \frac{\beta}{4}(x_q y_p^3 + 4x_q^3 y_p) - \frac{\gamma}{2}x \cdot y - i\frac{\gamma}{4}y \cdot y \quad (5.3.38)$$

and the \hbar term in the expansion is

$$\mathcal{H}^{(1)}(x, y) = i\frac{\gamma}{2}. \quad (5.3.39)$$

We now consider a cat state comprised of two Gaussian coherent states centred at $q = 4$ and $p = \pm 3$ in phase space with initial $B = iI$. As we have seen before in, the examples in Chapter 2 and Chapter 3, the Wigner function of such a cat state is composed of two Gaussians centred at $(4, \pm 3)$ in phase space, and a highly oscillatory interference pattern centred between the Gaussian peaks. By using our equations of motion for Z , B and α we can evolve each of the terms in the Wigner function and sum up the results to arrive at the semiclassical evolution of the cat state. We compare this evolution with the quantum dynamics in Figure 5.1.

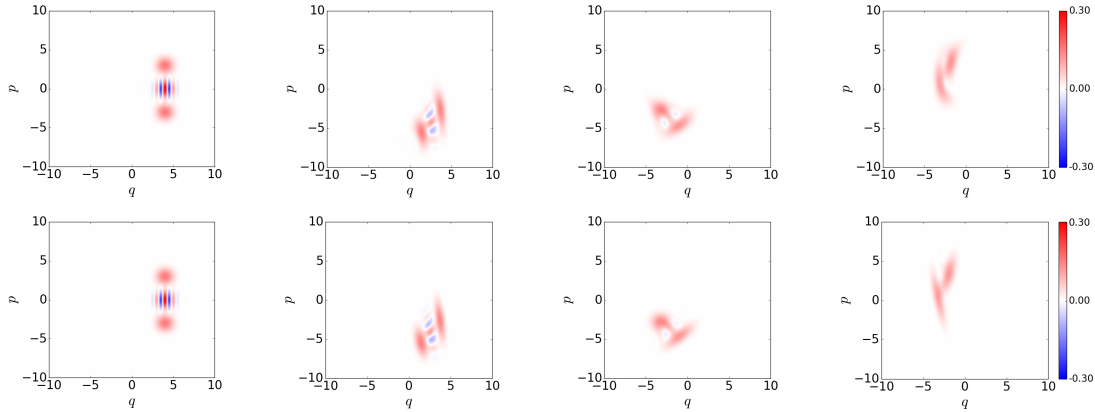


Figure 5.1: [12] The quantum (top) and semiclassical (bottom) dynamics of an initial cat state in an anharmonic potential with $\beta = 0.1$ and damping at a rate $\gamma = 0.3$. Times $t = 0, 0.5, 1.5, 2.5$ are shown from left to right.

If we compare the expectation values of the semiclassical position and momentum to the quantum results for larger times, we see that the two results begin to differ on longer timescales but still essentially resemble the quantum dynamics. This is shown in Fig. 5.2.

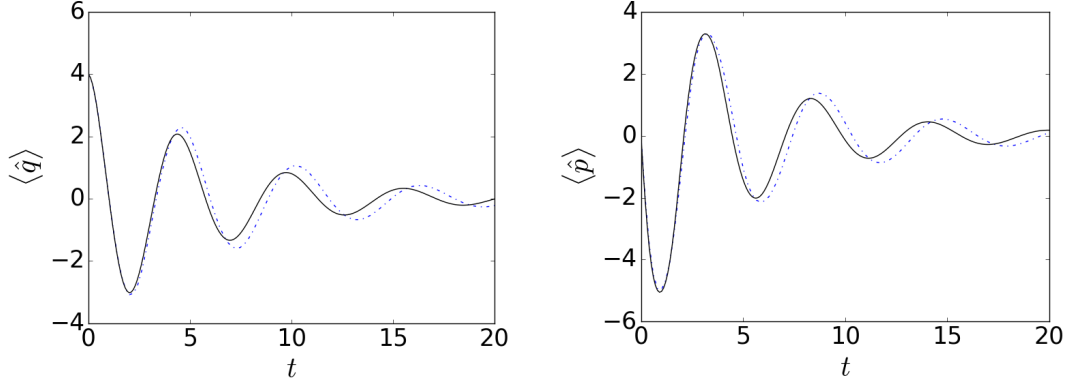


Figure 5.2: [12] Time evolution of the position (left) and momentum (right) expectation values of the cat state above. The quantum dynamics (black) are compared to the semiclassical results (blue dashed). Anharmonic parameter $\beta = 0.1$ and damping rate $\gamma = 0.3$.

5.4 Comparison to previous work

In the first sections of our paper [12] a similar looking result is determined for initial Wigner functions of the form

$$W(x) = \frac{\sqrt{\det G}}{(\pi\hbar)^n} e^{-\frac{1}{\hbar}(x-X) \cdot G(x-X)} \quad (5.4.1)$$

for $x = (q, p)$ where equations of motion for the centre $X = (Q, P)$ and the covariance matrix G

$$\dot{X} = \Omega \nabla H + \Omega \sum_k \text{Im}(L_k \nabla \bar{L}_k), \quad (5.4.2)$$

and

$$\dot{G} = \Lambda \Omega G - G \Omega \Lambda^T + 2G \Omega D \Omega G \quad (5.4.3)$$

are determined for

$$\Lambda := H'' + \sum_k \text{Im}(L_k \bar{L}_k'') + \sum_k \text{Im}(\nabla L_k \nabla \bar{L}_k^T) \quad (5.4.4)$$

and

$$D := \sum_k \text{Re}(\nabla L_k \nabla \bar{L}_k^T). \quad (5.4.5)$$

This result is determined by a more direct application of the Hepp-Heller method and the implications of this result are discussed more thoroughly, in particular the geometric interpretation of the Lindblad terms in the dynamical equations. In the case where the Lindblad operators are purely Hermitian or anti-Hermitian the flow generated by the

Lindblad terms vanishes, this results in decoherence but no dissipation in the semiclassical description which is a known and expected result [41]. In the case where the symbols L_k are holomorphic functions of $q \pm ip$, e.g. the heat bath operators we saw before, the flow can be written in terms of the gradient flow of the phase space function $\Gamma := \mp \frac{1}{2}|L|^2$. The results are also reformulated in the language of creation and annihilation operators, and applied to a set of examples including a description of cold atoms in optical lattices undergoing particle losses using an M mode Bose-Hubbard Hamiltonian.

While these results are very interesting in their own right, they are not our present focus and hence we only mention them in passing. It is important however that we show that the two approaches give equivalent and consistent evolution equations, i.e. that the set of equations (5.4.2-5.4.3) match the equations (5.3.31-5.3.34) we determined via the interpretation of the Lindblad equation as a Schrödinger equation on doubled phase space.

In the case of the doubled phase space approach we actually consider a more general initial Wigner function than (5.4.1), namely we introduce a linear term in the exponential in keeping with the generalised coherent state structure. If we consider $\mathcal{H}^{(0)}$ we see that the imaginary part is an *even* function of y , that is

$$\text{Im } \mathcal{H}^{(0)}(x, -y) = \text{Im } \mathcal{H}^{(0)}(x, y) \quad (5.4.6)$$

where $\text{Im } \mathcal{H}^{(0)}(x, 0) = 0$ and it is a strictly non-positive function. Similarly, we see the real part is an *odd* function of y

$$\text{Re } \mathcal{H}^{(0)}(x, -y) = -\text{Re } \mathcal{H}^{(0)}(x, y). \quad (5.4.7)$$

Using this one finds via direct computation that

$$\nabla \text{Re } \mathcal{H}^{(0)}(x, 0) = \left(0, \Omega \nabla_x H(x) + \Omega \sum_k \text{Im}(L_k(x) \nabla \bar{L}_k(x)) \right), \quad (5.4.8)$$

$$\nabla \text{Im } \mathcal{H}^{(0)}(x, 0) = (0, 0). \quad (5.4.9)$$

Plugging this into (5.3.31) we see that if $Y_0 = 0$ then $Y(t) = 0$ for all time, and $X(t)$ satisfies the same equation (5.4.2) found via the direct approach.

If we let $B = 2iG$ and use this in (5.3.32), then separating the Hessian matrix of $\mathcal{H}^{(0)}$ into real and imaginary parts at $y = 0$, we determine the same equation (5.4.3) for G .

Clearly then the equations (5.3.31 - 5.3.34) cover a more general class of initial conditions, in particular when $Y \neq 0$. This corresponds to a highly oscillatory initial Wigner function symptomatic of a very non-classical state. We saw that $\text{Im } \mathcal{H}^{(0)}$ has a global maximum at $y = 0$ and we see that the gradient part of equation (5.3.31) pushes the “momentum” part of the centre Y towards this maxima at zero, thereby inducing damping in these oscillations. If $\text{Im } \mathcal{H}^{(0)} < 0$ there is also an exponential damping induced by the $\mathcal{H}^{(0)}$ term in (5.3.34). Since the imaginary part is composed entirely of Lindblad terms we conclude that the coupling to the environment induces

rapid smoothing of highly oscillatory (non-classical) initial conditions. Hence we see the symptoms of the onset of decoherence as we would expect.

As mentioned before, the idea of using a doubled phase space approach to investigate the Lindblad equation is not a new one, and indeed it was investigated rather thoroughly by Brodier and Ozorio de Almeida [3] in the case of linear Lindblad operators written in the form

$$\hat{L}_k = l_k \cdot \hat{x} \quad (5.4.10)$$

for $l_k \in \mathbb{C}^{2n}$. Our results should mirror theirs in this case, but, as we will see, if we go beyond this linear case additional terms arise which are not covered in their theory.

The method of [3] starts by considering the characteristic function (2.5.20)¹

$$\chi_{\hat{\rho}}(t, y) := \text{tr} \left(\hat{\rho} e^{-\frac{i}{\hbar} y \cdot \hat{x}} \right). \quad (5.4.11)$$

If we compute the characteristic function of our initial wave packet (5.3.27) we find (see (2.7.31))

$$\chi(y) = N e^{\frac{i}{\hbar} [\frac{1}{2}(y-Y) \cdot (\mathbb{N} + i\mathbb{M})(y-Y) + X \cdot y]} \quad (5.4.12)$$

where we have defined the real symmetric matrices \mathbb{N} and \mathbb{M} via

$$-B^{-1} = \mathbb{N} + i\mathbb{M}. \quad (5.4.13)$$

The normalization can be determined using $\chi(0) = \text{tr} \hat{\rho}$. Here we have collected all the additional phase factors into the normalization for convenience since they will not effect the results.

In [3] they found the following set of equations for the evolutions of X, Y, \mathbb{N} and \mathbb{M} which we quote verbatim using their notation:

Proposition 5.4.1 (Brodier-Ozorio de Almeida [3]).

$$\dot{X}_t = \frac{\partial \mathcal{H}}{\partial y} + \mathbb{N}_t (\mathbb{M}_t)^{-1} \mathbb{D} Y_t, \quad \dot{Y}_t = -\frac{\partial \mathcal{H}}{\partial x} - (\mathbb{M}_t)^{-1} \mathbb{D} Y_t \quad (5.4.14)$$

$$\dot{\mathbb{N}}_t = -\mathbb{N}_t \frac{\partial^2 \mathcal{H}}{\partial x^2} \mathbb{N}_t + \mathbb{M}_t \frac{\partial^2 \mathcal{H}}{\partial x^2} \mathbb{M}_t + \frac{\partial^2 \mathcal{H}}{\partial y \partial x} \mathbb{N}_t + \mathbb{N}_t \frac{\partial^2 \mathcal{H}}{\partial x \partial y} - \frac{\partial^2 \mathcal{H}}{\partial y^2} \quad (5.4.15)$$

$$\dot{\mathbb{M}}_t = -\mathbb{M}_t \frac{\partial^2 \mathcal{H}}{\partial x^2} \mathbb{N}_t - \mathbb{N}_t \frac{\partial^2 \mathcal{H}}{\partial x^2} \mathbb{M}_t + \frac{\partial^2 \mathcal{H}}{\partial y \partial x} \mathbb{M}_t + \mathbb{M}_t \frac{\partial^2 \mathcal{H}}{\partial x \partial y} + \mathbb{D} \quad (5.4.16)$$

where $\mathbb{D} = \Omega (\text{Re } l (\text{Re } l)^T + \text{Im } l (\text{Im } l)^T) \Omega^T$.

To show that this set of equations matches the ones we found in Theorem 5.3.2 we use the result that

$$\mathcal{G}^{-1} = \begin{pmatrix} \mathbb{M} + \mathbb{N} \mathbb{M}^{-1} \mathbb{N} & -\mathbb{N} \mathbb{M}^{-1} \\ -\mathbb{M}^{-1} \mathbb{N} & \mathbb{M}^{-1} \end{pmatrix} \quad (5.4.17)$$

which can be shown by brute force computation, or by directly applying Proposition 3.2 in [14] with the choice of symplectic matrix $S = \Omega^{-1}$.

¹They use the name ‘‘Chord function’’.

If we consider linear Lindblad operators then $\text{Im } \mathbb{H}^{(0)} = -\frac{1}{2}y \cdot \mathbb{D}y$ and the equation of motion for Z can be split into an equation of motion for X and Y separately as

$$\dot{X} = \nabla_y \text{Re } \mathcal{H} + \mathbb{N}\mathbb{M}^{-1}\mathbb{D}Y, \quad \dot{Y} = -\nabla_x \text{Re } \mathcal{H} - \mathbb{M}^{-1}\mathbb{D}Y \quad (5.4.18)$$

matching with (5.4.14).

To determine the equations for \mathbb{N} and \mathbb{M} we use that

$$\dot{\mathbb{N}} + i\dot{\mathbb{M}} = B^{-1}\dot{B}B^{-1}. \quad (5.4.19)$$

Plugging this into (5.3.32) and separating real and imaginary parts, one arrives at

$$\dot{\mathbb{M}} + \mathbb{D} + \text{Re } \mathcal{H}_{yx}\mathbb{M} + \mathbb{M}\mathcal{H}_{xy} - \mathbb{M}\mathcal{H}_{xx}\mathbb{N} - \mathbb{N}\mathcal{H}_{xx}\mathbb{M} \quad (5.4.20)$$

and

$$\dot{\mathbb{N}} = -\mathcal{H}_{yy} + \mathcal{H}_{yx}\mathbb{N} + \mathbb{N}\mathcal{H}_{xy} + \mathbb{M}\mathcal{H}_{xx}\mathbb{M} - \mathbb{N}\mathcal{H}_{xx}\mathbb{N} \quad (5.4.21)$$

matching (5.4.16) and (5.4.15) respectively.

As mentioned, our approach allows the consideration of more general Lindblad operators than the linear ones considered in [3] or in the previous chapters of this thesis. In the case of these more general Lindblad operators, $\text{Im } \mathcal{H}^{(0)}$ will no longer be a quadratic form in y and instead will depend on both y and x . Hence, this will give rise to extra terms in the equations of motion for X, Y, \mathbb{M} and \mathbb{N} which are not captured by the results of [3]. If we consider the case where $\mathbb{N} = 0$ then we are in the regime of $B = \frac{1}{2}\mathbb{M}^{-1}$ which is just the G of equation (5.4.3) which clearly has terms involving second derivatives of the Lindblad operators.

5.5 Outlook

In this chapter, using the doubled phase space construction, we have determined a method for finding coherent state phase space solutions to the Lindblad equation for general Hamiltonians \hat{H} and Lindblad operators \hat{L}_k . In the context of this thesis as a whole, the obvious question one might ask is how can we relate these equations back to the study of decoherence we made in the linear and quadratic case? Which terms in the doubled Hamiltonian \mathcal{H} contribute to decoherence and which contribute to transport? How does this relate to the Hörmander condition, does the result, Theorem 3.4.9, hold and if so to what level of approximation? Do we see the same separation of timescales appear? It is hoped that using this more general result we can make concrete statements about the spread of decoherence in more general systems and environments but this is as of yet a mostly unexplored area of study.

If we restrict ourselves to the case of Linear Lindblads and quadratic Hamiltonians, we find that, using the form $\sum_k \bar{l}_k l_k^T = M + iN$ we used previously (see 2.6.26)

$$\mathcal{H}^{(0)}(x, y) = -x \cdot H''\Omega y + x \cdot \Omega N y - \frac{i}{2}y \cdot M y, \quad (5.5.1)$$

where $\sum_k \bar{l}_k l_k^T = M + iN$ as before. Note then that the derivatives are given by

$$\mathcal{H}_{xx}^{(0)} = 0, \quad \mathcal{H}_{xy}^{(0)} = A^T, \quad \mathcal{H}_{yx}^{(0)} = A, \quad \mathcal{H}_{yy}^{(0)} = -iM. \quad (5.5.2)$$

where $A = \Omega H'' + N\Omega$ as before.

Now, taking as before $B = 2iG$, we see that G satisfies

$$\dot{G} = -2GMG - GA - A^T G \quad (5.5.3)$$

and in particular if G is real, then it stays real. This means that B remains purely imaginary and hence \mathcal{G} has the block diagonal form:

$$\mathcal{G} = \begin{pmatrix} 2G & 0 \\ 0 & \frac{1}{2}G^{-1} \end{pmatrix}. \quad (5.5.4)$$

Importantly, this means that the equations for \dot{X} and \dot{Y} decouple into the equations

$$\dot{Z} = \begin{pmatrix} \dot{X} \\ \dot{Y} \end{pmatrix} = \begin{pmatrix} AX \\ -(A^T + 2GM)Y \end{pmatrix}. \quad (5.5.5)$$

The first of these is solved easily as $X = e^{At}X_0 = R_t X_0$ reproducing the motion of the centre $\bar{y}_{jk}(t)$ described in Lemma 3.2.5.

As for the rest of the terms, we claim that Y will be equivalent to the term $\xi_{jk}(t)$ and that the term describing decoherence, involving the matrix \tilde{C}_t , will arise from the imaginary part of the term $-\mathcal{H}^{(0)}(X, Y)$ in the equation for α (5.3.34).

The full connection between these two approaches, in particular how the results on timescales and Hörmander's condition generalise to general Hamiltonians and Lindblad operators, is still very much an open area of study and further work will be needed to describe the spread of decoherence in these more general situations.

Chapter 6

Conclusion

The overall theme of this thesis was focussed on using semiclassical methods arising from the phase space picture of quantum mechanics to investigate decoherence. In particular, we were interested in investigating the Lindblad equation on phase space

$$i\hbar \frac{\partial \rho}{\partial t} = H \star \rho - \rho \star H + i \sum_j L_j \star \rho \star \bar{L}_j - \frac{1}{2} \bar{L}_j \star L_j \star \rho - \frac{1}{2} \rho \star \bar{L}_j \star L_j \quad (6.0.1)$$

with a particular focus on the evolution of Gaussian coherent states.

In Chapter 3 we restricted ourselves to the situation where our Hamiltonian $H(x)$ was at most quadratic in $x = (q, p)$, and our Lindblads $L_k(x)$ were at most linear in x . In this situation the Lindblad equation becomes an exact second order equation on phase space which we could write in terms of a set of vector fields $X_0, X_j, j = 1, \dots, 2K$ as

$$\partial_t \rho = X_0 \rho + \nabla \cdot X_0 \rho + \frac{\hbar}{2} \sum_{k=1}^{2K} X_k^2 \rho. \quad (6.0.2)$$

We saw that the spread of decoherence due to the environment in this system was intimately related to a condition from the theory of PDEs known as the Hörmander condition[20]. In particular, in Theorem 3.4.9 we showed that if the vector fields $X_0, X_j, j = 1, \dots, 2K$ satisfied the Hörmander condition then the effect of the environment spread to all parts of the system, and it experienced full decoherence.

Further than this, the Hörmander condition was shown to provide a natural orthogonal decomposition of our phase space \mathbb{R}^{2n} into a set of orthogonal subspaces W_i . We showed that these subspaces encoded the timescales upon which the effect of the environment spread throughout the system so that a state in W_0 would decohere on a faster timescale than a state in W_1 and so on. We also showed that if Hörmander's condition is *not* satisfied, then there exists a protected subspace W_{df} which does not experience decoherence.

We also determined an explicit solution to the Lindblad equation for initially Gaussian coherent states as well as a formula for the Hilbert-Schmidt norm of the evolved state. Using these results we were able to show this separation of timescales and the

existence of protected subspaces explicitly by centring superpositions of coherent states in the corresponding subspaces for a set of simple examples.

In Chapter 4 we investigated these results on the spread of decoherence for a larger class of examples, namely networks of interacting harmonic oscillators. By considering the simple case of a chain of harmonic oscillators in a heat bath environment we saw we could reduce the Hörmander condition to checking whether the product of powers of a matrix \mathbb{H} , describing the overall internal structure of the system, and a vector \mathbb{c} , describing which oscillators were coupled to the environment, were linearly independent. In particular, because we chose to consider a heat bath environment, we reduced our problem to an N dimensional rather than $2N$ dimensional calculation.

By changing the oscillator which was coupled to the environment, we saw that the spread of decoherence changed dramatically. When coupling to the first oscillator decoherence would proceed down the chain to each oscillator in turn as one might expect, but if you coupled to a middle oscillator the spaces W_i become more complicated and in some cases there existed a protected subspace W_{df} . By investigating this more thoroughly we saw that if $N + 1$ was prime, where N is the length of the chain, there would be no protected subspaces. However if $N + 1$ was non-prime there would be a protected subspace.

We also investigated two other simple examples, namely the loop and the star. In both cases we saw that there was no single oscillator to which you could couple the environment for which Hörmander's condition would not fail. That is, there was always a protected subspace.

In Theorem 4.2.1 we provided an algorithm which could be used to investigate more complicated networks where some of the simplifications we were able to exploit for our simple harmonic oscillator networks no longer held. However there is still a lot that could yet be said about these networks as we discussed at the end of the chapter. In particular we could try to extend these ideas to model more physically realistic systems where all oscillators are coupled to a weak environment, but one is coupled much more strongly. In this situation we postulate that we would see 'weakly protected' subspaces which on short timescales do not experience decoherence. Beyond this, the underlying symmetries of the networks that determine the structure of the subspaces W_i and W_{df} are not well understood and this would be a further direction of study.

Finally, in Chapter 5 we tried to relax the restriction to quadratic Hamiltonians and linear Lindblads we had taken in the previous two chapters and investigate coherent state solutions of the full Lindblad equation. To do this we reinterpreted the phase space Lindblad equation as a Schrödinger equation on a doubled phase space of the form

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{\mathcal{H}}(\hat{x}, \hat{y})\psi \quad (6.0.3)$$

where we took our Weyl symbol ρ to initially be a coherent state $\rho = \psi_Z^B(x)$ on this doubled phase space centred at $Z = (X, Y)$. This Hamiltonian $\hat{\mathcal{H}}$ was shown to be manifestly non-Hermitian, and hence we were able to apply recent results from the study of non-Hermitian Schrödinger equations [13][14] to determine a set of evolution equations

for the centre Z , the covariance matrix B and the overall phase α of the coherent state $\psi_Z^B(x)$ in Theorem 5.3.2. In particular this method allows us to investigate off-diagonal terms in the Wigner function corresponding to highly non-classical states. While this theorem allows us to investigate the evolution of Gaussian states under the Lindblad equation for general Hamiltonians and Lindblads, how we can relate it to the previous results in this thesis on decoherence is an emerging area of study.

Appendices

Appendix A

A specific Gaussian Integral

Consider the integral of the form

$$I(x, \delta\xi, \mathcal{A}, \mathcal{B}) = \frac{1}{(2\pi\hbar)^n} \int_{\mathbb{R}^{2n}} e^{\frac{i}{\hbar}x \cdot \xi} e^{-\frac{1}{2\hbar}(\xi - \delta\xi) \cdot \mathcal{A}(\xi - \delta\xi)} e^{-\frac{1}{2\hbar}\xi \cdot \mathcal{B}\xi} d\xi. \quad (\text{A.0.1})$$

Here we consider \mathcal{A}, \mathcal{B} to be real, symmetric $2n \times 2n$ matrices such that $\mathcal{A} + \mathcal{B} > 0$, $\hbar > 0$ and $x, \delta\xi \in \mathbb{C}^{2n}$.

These sorts of integrals can be reduced to the well known Fourier transform of a Gaussian

$$\frac{1}{(2\pi\hbar)^{d/2}} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar}y \cdot \xi} e^{-\frac{1}{2\hbar}\xi \cdot \Gamma \xi} d\xi = \frac{1}{\sqrt{\det \Gamma}} e^{-\frac{1}{2\hbar}y \cdot \Gamma^{-1}y} \quad (\text{A.0.2})$$

where Γ is a symmetric and strictly positive $d \times d$ matrix, $\hbar > 0$ and $y \in \mathbb{C}^d$. Zworski provides a good reference for this and many other Gaussian Fourier transform results [51].

We now have the following result

Lemma A.0.1. *The integral $I(x, \delta\xi, \mathcal{A}, \mathcal{B})$ is given explicitly by*

$$I(x, \delta\xi, \mathcal{A}, \mathcal{B}) = \frac{1}{\sqrt{\det(\mathcal{A} + \mathcal{B})}} e^{-\frac{1}{2\hbar}\delta\xi \cdot \mathcal{B}(\mathcal{A} + \mathcal{B})^{-1}\mathcal{A}\delta\xi} e^{\frac{i}{\hbar}\delta\xi \cdot \mathcal{A}(\mathcal{A} + \mathcal{B})^{-1}x} e^{-\frac{1}{2\hbar}x \cdot (\mathcal{A} + \mathcal{B})^{-1}x} \quad (\text{A.0.3})$$

Proof. We can write the exponent of the integrand (minus the Fourier part) as

$$(\xi - \delta\xi) \cdot \mathcal{A}(\xi - \delta\xi) + \xi \cdot \mathcal{B}\xi = -2(\mathcal{A}\delta\xi) \cdot \xi + \xi \cdot (\mathcal{A} + \mathcal{B})\xi + \delta\xi \cdot \delta\xi \quad (\text{A.0.4})$$

and using this we can write $I(x, \delta\xi, \mathcal{A}, \mathcal{B})$ in the form of the Fourier integral above

$$I(x, \delta\xi, \mathcal{A}, \mathcal{B}) = \frac{1}{(2\pi\hbar)^{d/2}} \int_{\mathbb{R}^d} e^{\frac{i}{\hbar}y \cdot \xi} e^{-\frac{1}{2\hbar}\xi \cdot \Gamma \xi} d\xi e^{-\frac{1}{2\hbar}\delta\xi \cdot \mathcal{A}\delta\xi} \quad (\text{A.0.5})$$

where we have defined

$$y = x - i\mathcal{A}\delta\xi, \quad \Gamma = (\mathcal{A} + \mathcal{B}). \quad (\text{A.0.6})$$

Hence, the Fourier result above gives

$$I(x, \delta\xi, \mathcal{A}, \mathcal{B}) = \frac{1}{\sqrt{\det(\mathcal{A} + \mathcal{B})}} e^{-\frac{1}{2\hbar} y \cdot (\mathcal{A} + \mathcal{B})^{-1} y} e^{-\frac{1}{2\hbar} \delta\xi \cdot \mathcal{A} \delta\xi} \quad (\text{A.0.7})$$

and inserting the y defined above we get

$$\delta\xi \cdot \mathcal{A} \delta\xi + y \cdot (\mathcal{A} + \mathcal{B})^{-1} y = \delta\xi \cdot [\mathcal{A} - \mathcal{A}(\mathcal{A} + \mathcal{B})^{-1} \mathcal{A}] \delta\xi - 2i \delta\xi \cdot \mathcal{A}(\mathcal{A} + \mathcal{B})^{-1} x + x \cdot (\mathcal{A} + \mathcal{B})^{-1} x. \quad (\text{A.0.8})$$

Combining this with

$$\mathcal{A} - \mathcal{A}(\mathcal{A} + \mathcal{B})^{-1} \mathcal{A} = (\mathcal{A} + \mathcal{B} - \mathcal{A})(\mathcal{A} + \mathcal{B})^{-1} \mathcal{A} = \mathcal{B}(\mathcal{A} + \mathcal{B})^{-1} \mathcal{A} \quad (\text{A.0.9})$$

gives

$$I(x, \delta\xi, \mathcal{A}, \mathcal{B}) = \frac{1}{\sqrt{\det(\mathcal{A} + \mathcal{B})}} e^{-\frac{1}{2\hbar} \delta\xi \cdot \mathcal{B}(\mathcal{A} + \mathcal{B})^{-1} \mathcal{A} \delta\xi} e^{\frac{i}{\hbar} \delta\xi \cdot \mathcal{A}(\mathcal{A} + \mathcal{B})^{-1} x} e^{-\frac{1}{2\hbar} x \cdot (\mathcal{A} + \mathcal{B})^{-1} x} \quad (\text{A.0.10})$$

completing the proof. □

Appendix B

A specific trigonometric identity

For $k, l \in \mathbb{N}$ and $n \in \mathbb{N}$ such that $k, l \leq n$ consider the sum

$$A_{kl} = \sum_{j=1}^n \sin\left(\frac{k\pi}{n+1}j\right) \sin\left(\frac{l\pi}{n+1}j\right). \quad (\text{B.0.1})$$

Proposition B.0.1.

$$A_{kl} = \frac{n+1}{2} \delta_{kl}. \quad (\text{B.0.2})$$

Proof. We start by noting that

$$A_{kl} = \frac{1}{2} \sum_{j=1}^n \cos\left(\frac{(k-l)\pi}{n+1}j\right) - \cos\left(\frac{(k+l)\pi}{n+1}j\right) \quad (\text{B.0.3})$$

and letting $\theta_{\pm} = \frac{(k \pm l)\pi}{n+1}$ we have

$$A_{kl} = \frac{1}{2} \sum_{j=1}^n \cos(j\theta_-) - \cos(j\theta_+). \quad (\text{B.0.4})$$

We now recall the following trigonometric identity due to Lagrange [38]:

$$\sum_{j=1}^n \cos(j\theta) = \frac{1}{2} \left[\frac{\sin((n + \frac{1}{2})\theta)}{\sin(\frac{1}{2}\theta)} - 1 \right] \quad (\text{B.0.5})$$

which holds when $\theta \neq 0$.

Note as well that

$$\begin{aligned} \sin\left((n + \frac{1}{2})\theta\right) &= \sin\left((n+1)\theta - \frac{1}{2}\theta\right) \\ &= \sin((n+1)\theta) \cos\left(\frac{1}{2}\theta\right) - \cos((n+1)\theta) \sin\left(\frac{1}{2}\theta\right). \end{aligned}$$

and hence the Lagrange identity reduces to

$$\sum_{j=1}^n \cos(j\theta) = \frac{1}{2} \left[\sin((n+1)\theta) \cot\left(\frac{1}{2}\theta\right) - \cos((n+1)\theta) - 1 \right]. \quad (\text{B.0.6})$$

We start by considering the diagonal case, when $k = l$. In this situation $\theta_- = 0$ and $\theta_+ = 2\pi k$. Then

$$\begin{aligned} A_{kk} &= \frac{1}{2} \sum_{j=1}^n (1 - \cos(j\theta_+)) \\ &= \frac{n}{2} - \frac{1}{4} \left[\frac{\sin((n+\frac{1}{2})\theta_+)}{\sin(\frac{1}{2}\theta_+)} - 1 \right] \\ &= \frac{n}{2} - \frac{1}{4} \left[\sin(2k\pi) \cot\left(\frac{k\pi}{n+1}\right) - \cos(2k\pi) - 1 \right] \\ &= \frac{n}{2} - \frac{1}{4} [-2] \\ &= \frac{n+1}{2}, \end{aligned}$$

since $\sin(2k\pi) = 0$ and $\cos(2k\pi) = 1$ for all k .

If we now consider $k \neq l$, then the same method follows but we have to expand both terms.

$$\begin{aligned} A_{kl} &= \frac{1}{4} \left[\left[\frac{\sin((n+\frac{1}{2})\theta_-)}{\sin(\frac{1}{2}\theta_-)} - 1 \right] - \left[\frac{\sin((n+\frac{1}{2})\theta_+)}{\sin(\frac{1}{2}\theta_+)} - 1 \right] \right] \\ &= \frac{1}{4} \left[\sin((k-l)\pi) \cot\left(\frac{1}{2}\theta_-\right) - \cos((k-l)\pi) - \sin((k+l)\pi) \cot\left(\frac{1}{2}\theta_+\right) + \cos((k+l)\pi) \right] \\ &= \frac{1}{4} [\cos((k+l)\pi) - \cos((k-l)\pi)] \\ &= \frac{1}{4} [\cos k\pi \cos l\pi - \sin k\pi \sin l\pi - \cos k\pi \cos l\pi - \sin k\pi \sin l\pi] \\ &= -\frac{1}{2} \sin k\pi \sin l\pi \\ &= 0 \end{aligned}$$

since $\sin(m\pi) = 0$ for all $m \in \mathbb{Z}$.

□

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